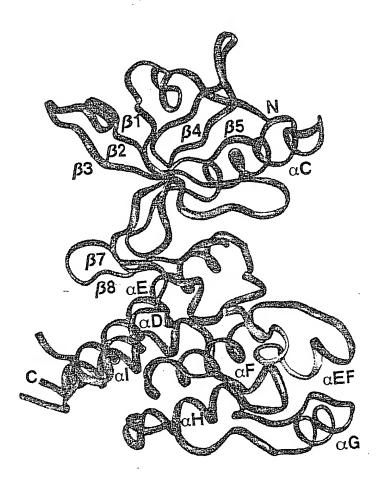
1/67	<u>u</u>	1010 605 1114	1004
863 509 1025 856 622 	916 681 953 586	- 61/	<u> </u>
8121-812		TO TO YES	
1 1 1 1 1 1 1 1	55	OE VS.	000
AE AE CK	200 1>>	KO H	
KGE KSP KSP KSP KSP KSP KSP		ADM ADM TLE SSF	JAH Jah
GLS GLD GLD GLD GLS WV	λ λ λ λ λ λ λ	NYON PEL	SEGUL SEGUL
SAF SAF TAY SPLN	GPL GPL	NN XX	7777 7777 7777 7777 7777 777
92 71 A A G G V C G G V C G G V C G G C C C C C C	X-0000	SFE	SDG SDG LSD
ding GOV GON GEN GEN GON	V SF V SF V SF V SF V SF V SF V SF V SF	VIL	EED KNL
Day Ding Ding Ding Ding Ding Ding Ding Ding	LLG/ LLG/ LLG/ Dme	HSY.	VEE SEV
Jide-b loop GRG/ LGRG LGRG LGRG LGRG LGRG	0 to	EST	T SD WLD
MDPDELPLDEHCERLPYDASKWEFPRDRLKLGKPLGRGAFGQVE ADAFGIDKTATCR MLAGVSEY - ELP - EDPRWELPRDRLYLGKPLGEGCFGQVL AEA1 GLDKDKPNRVT MLAGVSEY - ELP - EDPRWELPRDRLYLGKPLGEGCFGQVL AEA1 KKSPTCR MLAGVSEY - ELP - EDPRWELPRDRLYLGKSLGRGAFGKVQASAFGIKKSPTCR MLAGVSEY	63 TVAVKMLKEGATHSEHRALMSELKILIHIGHKNIINLLGAUITGOPTLVVMELMAYGN TVAVKMLKSDATEKDLSDLISEMEMMKMIGKHKNIINVRLLGVSK-GOPTLVVMELMYGYGN KVAVKMLKSDATEKDLSDLISEMEMMKGFTCH-HVVRLLGACTKOGGPLMVIVEYCFYGD RVAVKTVNESASLRERIEFLNEASVMKGFTCH-HVVRLLGACTK-SGPIYIITEYCFYGD RVAVKTVNESASLRERIEFLNITHIGPHLNIVNLLGACTK-SGPIYIITEYCFYGD TVAVKMLKEGATASEYKALMTELKIMTHLGPHLNIVNLLGACTK-SGPIYIITEYCFYGD KVAVKMLKFTARSSEKQALMSELKIMTHLGPHCNIVNLLGACTK-SGPIYIITEYCFYGD	αD LSTYL RSKRNEF V P YKTKGARFROGKDY VG	AIPVDLKRRLDSITSSQSSASSGFVEERS COLL PSHING RPPPTLOEM LOWNER PROBLISYSF STY SECTOR SE
B1 B1 DADALVLGK PRDRLVLGK ARERITLL R PRDGLVLGK PRDGLVLGK PRDGLVLGK PRDGLVLGR	IGKI IGKI IGH IGP IGP	KAME	Y KK
D J H J H J H J H J H J H J H J H J H J	AKM AKM ATT K	KD KKE KKE	SSGI PAS
FPR	SVAN X	AEPI KELL	SAS SFA YDRI
A WE HER	SEL SEM NEA TEL ISEL	ARF LLIM CPKI	SOS
αΕ ASK EDPF PDI PDI PDI SASI	ALM PL I PL I ALN	TKG YN-	178 3VT8 51010
	EYK EYK EKC	PYK EYC SI	ISAX SULDS SULDS
P C C E R C C C C C C C C C C C C C C C C	TEK SLR TAS TAS	EFV PGL EA ILFF ISFL	KAR KRPI KKPI
EAC - VER -	ESA EGA EGA PTA	NAN ARR GRACA SKAC JRNS	VDL SOGN
PLD	ALK MLK MLK MLK	LAS LAS LAS LKS 1LKS	A IP
MLA	AKKAKA AKKA AKA A AKA A A A A A A A A A A A A A A A A A A A	ANY KSY KNY	\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \
MOP	リアグロトス	\\\—\\	954 587 1096 947 742
806 P 456 978 799 576	864 510 1026 857 623	924 569 1084 917 682	
		- R2	/EGF - R2 -GFR1 I RK /EGF - R1 >DGFR0
- R2	:-R2 31 F-R1 FR0	/EGF - F GFR1 RK /EGF -	SEGF SFR SFR SFR SFR DGF
EGE-R2 GFR1 RK EGF-R1 DGFR0	EGF-F GFR1 RK EGF- DGFR	16. 19. 10. 10.):
ПОСТ			

F1G. 1b

•	2/67	i O
1070 665 1174 1064 860	923 568 1083 916 681	1171 765 1274 1165 961
catalytic loop B3 B4 Catalytic loop B7 B8 Catalytic loop 1011 QVAKGMEFDLASRKC HRDLAARN LLSEKNVVKICDFGLARD YKDPDYVRKGDARLPVK 1011 QVAKGMEFDLASRKC HRDLAARNVLVTEDNVMKIADFGLARD YFTDYYRKGGKGLLPVR 606 QVARGMEYSLASKKC HRDLAARNCMVAHDFTVKIGDFGLARD YKNPDYVRKGDTRLPVK 610 QVARGMEY-LNAKKFVHRDLAARN LLSENNVVKIDDFGLARD YKNPDYVRKGSTFLPVK 611	1005 801 107 666 117	113 725 123 123 113
лан - 82 2 F - 82 3 F В 1	EGF-R1 5GFRα 5GF-R2 3FR1 RK RK	EGF-R2 GFR1 BK EGF-R1 DGFR0

FIG. 2a



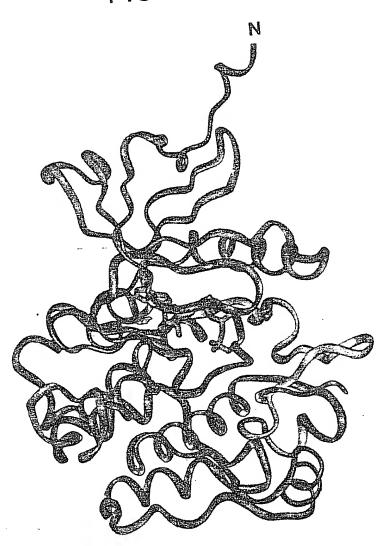
VEGFR2D50P

FIG. 2b



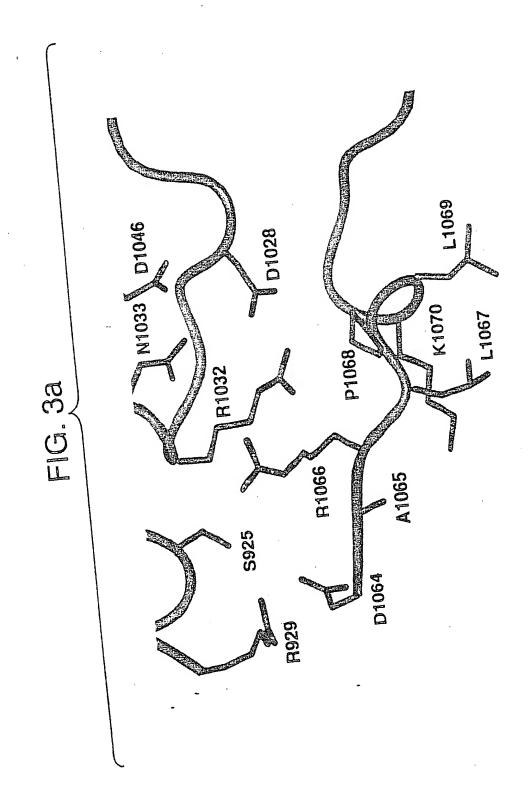
FGFR1

FIG. 2c

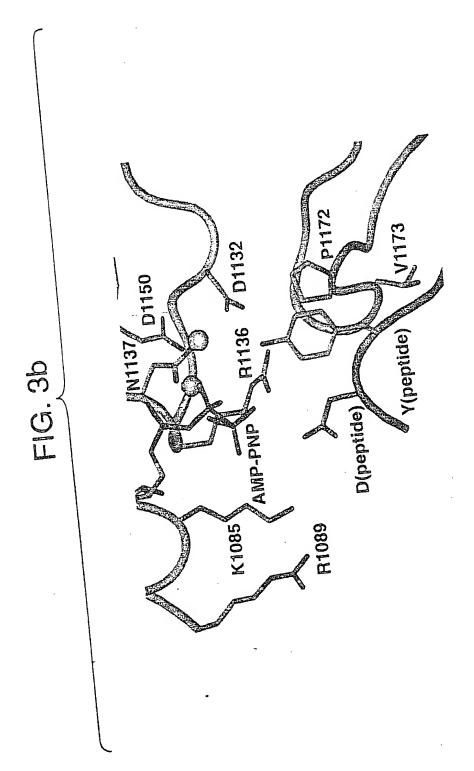


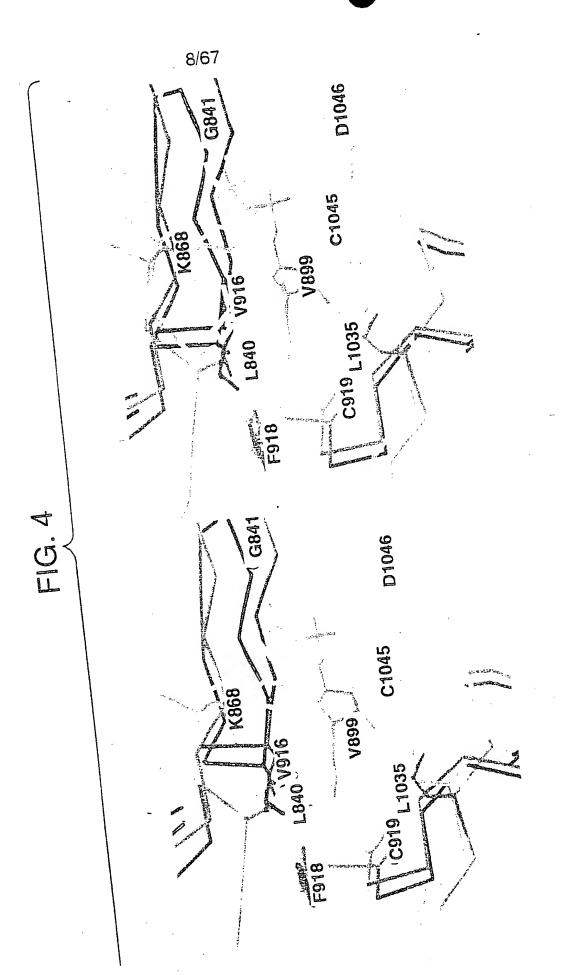
IRKP

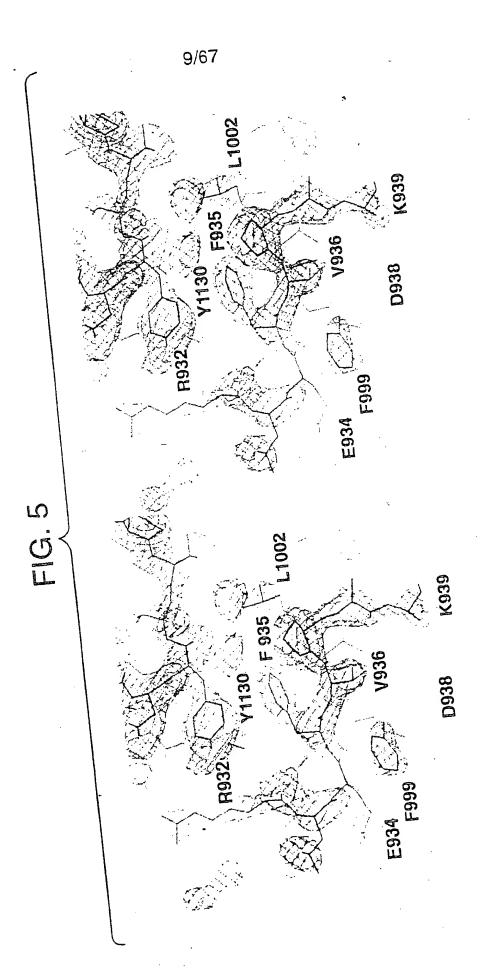




1100







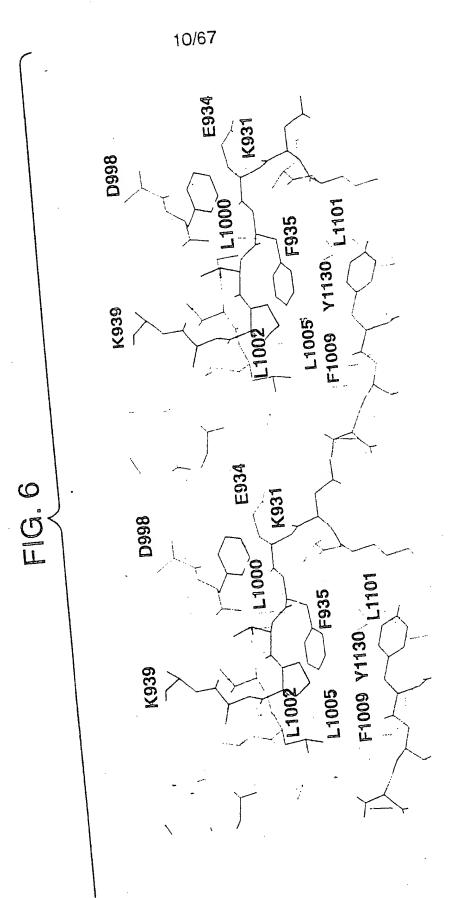


FIG. 7(1)

1 CB LEU 820 **ATOM** 2 CG LEU 820 **ATOM** 3 CD1 LEU 820 **ATOM** 4 CD2 LEU 820 ATOM 5 C LEU 820 ATOM 6 O LEU 820 ATOM 9 N LEU 820 **ATOM** 11 CA LEU 820 **ATOM** 12 N PRO 821 **ATOM** 13 CD PRO 821 ATOM 14 CA PRO 821 **ATOM** 15 CB PRO 821 **MOTA** 16 CG PRO 821 **ATOM** 17 C PRO 821 **ATOM** 18 O PRO 821 ATOM 19 N TYR 822 ATOM 21 CA TYR 822 **ATOM** 22 CB TYR 822 **ATOM** 23 CG TYR-822 **ATOM** 24 CD1 TYR 822 **ATOM** 25 CE1 TYR 822 **ATOM** 26 CD2 TYR 822 ATOM 27 CE2 TYR 822 ATOM 28 CZ TYR 822 ATOM 29 OH TYR 822 ATOM 31 C TYR 822 **ATOM** 32 O TYR 822 ATOM 33 N ASP 823 ATOM 35 CA ASP 823 ATOM 36 CB ASP 823 **ATOM** 37 CG ASP 823 **ATOM** 38 OD1 ASP 823 ATOM 39 OD2 ASP 823 ATOM 40 C ASP 823 ATOM 41 O ASP 823 ATOM 42 N ALA 824 ATOM 44 CA ALA 824 ATOM 45 CB ALA 824 ATOM 46 C ALA 824 ATOM 47 O ALA 824 ATOM

49.908 45.905 17.938 1.00 48.95 50.568 45.069 16.833 1.00 43.57 50.004 45.358 15.456 1.00 43.59 52.066 45.345 16.886 1.00 47.45 49.216 48.321 17.530 1.00 48.14 48.196 48.587 18.187 1.00 52.58 50.481 47.725 19.581 1.00 53.68 50.302 47.387 18.117 1.00 50.63 49.435 48.842 16.306 1.00 41.32 50.680 48.870 15.520 1.00 45.54 48.465 49.733 15.700 1.00 31.06 49.067 49.985 14.352 1.00 28.89 50.509 50.148 14.734 1.00 43.44 47.123 49.165 15.569 1.00 26.14 46.948 47.970 15.374 1.00 26.03 46.154 50.024 15.776 1.00 16.25 44.799 49.643 15.582 1.00 18.88 44.061 49.519 16.916 1.00 17.42 42.584 49.316 16.728 1.00 18.46 41.674 50.341 17.047 1.00 21.12 40.314 50.206 16.812 1.00 13.80 42.086 48.144 16.175 1.00 12.24 40.714 47.997 15.951 1.00 13.44 39.838 49.028 16.268 1.00 14.38 38.480 48.887 16.073 1.00 19.73 44.253 50.760 14.705 1.00 16.93 44.172 51.904 15.112 1.00 20.70 44.054 50.456 13.439 1.00 15.20 43.509 51.418 12.506 1.00 13.55 43.856 50.945 11.091 1.00 11.37 43.456 51.933 10.016 1.00 16.45 42.546 52.754 10.258 1.00 21.86 44.022 51.854 8.904 1.00 12.33 41.983 51.489 12.738 1.00 14.14 41.224 50.722 12.172 1.00 19.73 41.539 52.415 13.572 1.00 11.88 40.126 52.554 13.876 1.00 14.80 39.928 53.610 14.973 1.00 12.02 39.259 52.893 12.658 1.00 19.09 38.062 52.610 12.641 1.00 23.54

FIG. 7(2)

48 N SER 825 **ATOM** 50 CA SER 825 **ATOM** 51 CB SER 825 **ATOM** 52 OG SER 825 ATOM 54 C SER 825 ATOM 55 O SER 825 **ATOM** 56 N LYS 826 **ATOM** 58 CA LYS 826 **ATOM** 59 CB LYS 826 ATOM 60 CG LYS 826 **ATOM** 61 CD LYS 826 **ATOM** 62 CE LYS 826 **ATOM** 63 NZ LYS 826 **ATOM** 67 C LYS 826 **ATOM** 68 O LYS 826 ATOM 69 N TRP 827 **ATOM** 71 CA TRP 827 **ATOM** 72 CB TRP 827 **ATOM** 73 CG TRP 827 **ATOM** 74 CD2 TRP 827 **ATOM** 75 CE2 TRP 827 **ATOM** 76 CE3 TRP 827 **ATOM** 77 CD1 TRP 827 **ATOM** 78 NE1 TRP 827 **ATOM** 80 CZ2 TRP 827 **ATOM** 81 CZ3 TRP 827 **ATOM** 82 CH2 TRP 827 **ATOM** 83 C TRP 827 **ATOM** 84 O TRP 827 **ATOM** 85 N GLU 828 ATOM 87 CA GLU 828 **ATOM** 88 CB GLU 828 **ATOM** 89 CG GLU 828 **ATOM** 90 CD GLU 828 **ATOM** 91 OE1 GLU 828 **ATOM** 92 OE2 GLU 828 **ATOM** 93 C GLU 828 -**ATOM** 94 O GLU 828 **ATOM** 95 N PHE 829 ATOM 97 CA PHE 829 **ATOM** 98 CB PHE 829 ATOM 99 CG PHE 829 **ATOM**

39.857 53.496 11.635 1.00 18.25 39.118 53.867 10.450 1.00 12.65 9.543 1.00 11.88 40.023 54.678 39.315 55.003 8.370 1.00 20.94 9.746 1.00 12.30 38.669 52.594 9.317 1.00 14.94 37.543 52.461 9.642 1.00 14.98 39.557 51.633 8.988 1.00 22.45 39.188 50.396 40.445 49.660 8.483 1.00 16.46 7.820 1.00 23.00 40.091 48.370 6.657 1.00 26.19 40.962 48.071 7.092 1.00 35.70 42.391 48.041 5.891 1.00 40.17 43.272 48.003 9.839 1.00 21.47 38.324 49.437 37.363 48.850 9.336 1.00 22.56 38.589 49.376 11.144 1.00 20.96 37.917 48.406 11.996 1.00 16.87 38.974 47.620 12.785 1.00 18.53 39.942 46.898 11.910 1.00 12.95 39.643 45.810 11.029 1.00 9.73 40.795 45.562 10.274 1.00 9.36 38.505 45.038 10.801 1.00 11.54 41.233 47.231 11.684 1.00 12.87 41.753 46.440 10.689 1.00 10.49 40.848 44.565 9.299 1.00 12.36 38.556 44.053 9.826 1.00 10.55 39.718 43.830 9.087 1.00 11.88 36.830 48.795 12.953 1.00 17.75 35.985 47.951 13.271 1.00 15.08 36.855 50.043 13.416 1.00 16.92 35.908 50.518 14.413 1.00 19.52 36.289 51.920 14.885 1.00 17.10 35.581 52.363 16.148 1.00 12.70 36.106 51.707 17.400 1.00 21.57 37.219 51.118 17.386 1.00 21.15 35.402 51.819 18.426 1.00 22.43 34.494-50.510 13.910 1.00 20.94 34.245 51.024 12.818 1.00 26.92 33.569 49.990 14.734 1.00 21.12 32.138 49.880 14.391 1.00 17.93 31.791 48.400 14.160 1.00 16.42 30.384 48.164 13.669 1.00 20.17

FIG. 7(3)

100 CD1 PHE 829 MOTA 101 CD2 PHE 829 ATOM 102 CE1 PHE 829 ATOM 103 CE2 PHE 829 ATOM 104 CZ PHE 829 ATOM 105 C PHE 829 **ATOM** 106 O PHE 829 ATOM 107 N PRO 830 **ATOM** 108 CD PRO 830 ATOM 109 CA PRO 830 ATOM 110 CB PRO 830 **ATOM** 111 CG PRO 830 ATOM 112 C PRO 830 **ATOM** 113 O PRO 830 ATOM 114 N ARG 831 **ATOM** 116 CA ARG 831 ATOM 117 CB ARG 831 ATOM 118 CG ARG 831. ATOM 119 CD ARG 831 ATOM 120 NE ARG 831 **ATOM** 122 CZ ARG 831 **ATOM** 123 NH1 ARG 831 ATOM 126 NH2 ARG 831 ATOM 129 C ARG 831 **ATOM** 130 O ARG 831 **ATOM** 131 N ASP 832 **ATOM** 133 CA ASP 832 ATOM 134 CB ASP 832 ATOM 135 CG ASP 832 **ATOM** 136 OD1 ASP 832 **ATOM** 137 OD2 ASP 832 **ATOM** 138 C ASP 832 ATOM 139 O ASP 832 **ATOM** 140 N ARG 833 **ATOM** 142 CA ARG 833 ATOM 143 CB ARG 833 **ATOM** 144 CG ARG 833 ATOM 145 CD ARG 833 **ATOM** 146 NE ARG 833 ATOM 148 CZ ARG 833 **ATOM** 149 NH1 ARG 833 **ATOM** 152 NH2 ARG 833 ATOM 155 C ARG 833 **ATOM**

30.020 48.484 12.363 1.00 21.31 29.415 47.612 14.516 1.00 23.04 28.712 48.254 11.921 1.00 18.76 28.093 47.375 14.071 1.00 15.20 27.750 47.692 12.792 1.00 17.17 31.310 50.495 15.533 1.00 14.65 31.574 50.211 16.686 1.00 16.15 30.270 51.298 15.224 1.00 13.29 29.707 51.633 13.901 1.00 11.63 29.481 51.918 16.292 1.00 14.76 28.636 52.948 15.565 1.00 13.82 28.414 52.364 14.252 1.00 14.42 28.629 51.005 17.098 1.00 19.79 27.750 50.339 16.562 1.00 26.60 28.830 51.060 18.410 1.00 18.39 28.085 50.246 19.335 1.00 14.56 28.469 50.580 20.743 1.00 11.53 29.808 50.050 21.092 1.00 12.65 30.117 50.265 22.554 1.00 12.46 31.261 51.148 22.584 1.00 20.55 32.469 50.756 22.885 1.00 12.04 32.688 49.518 23.234 1.00 23.80 33.467 51.501 22.526 1.00 23.84 26.625 50.415 19.174 1.00 18.55 25.852 49.561 19.607 1.00 25.61 26.221 51.517 18.552 1.00 25.32 24.794 51.734 18.354 1.00 29.47 24.393 53.230 18.408 1.00 34.15 24.817 54.036 17.174 1.00 33.50 25.519 53.528 16.280 1.00 34.09 24.422 55.216 17.110 1.00 41.48 24.230 51.000 17.139 1.00 27.13 23.023 50.905 16.991 1.00 28.08 25.104 50.466 16.290 1.00 24.18 24.684 49.695 15.134 1.00 19.93 25.661 49.902 14.011 1.00 25.94 25.313 51.073 13.158 1.00 38.97 25.929 50.901 11.766 1.00 53.19 25.525 51.930 10.807 1.00 63.47 25.419 53.229 11.087 1.00 70.42 25.040 54.080 10.139 1.00 74.08 25.695 53.690 12.306 1.00 72.08 24.656 48.218 15.498 1.00 18.62

FIG. 7(4)

ATOM 156 O ARG 833 ATOM 157 N LEU 834 159 CA LEU 834 **ATOM** 160 CB LEU 834 ATOM 161 CG LEU 834 ATOM 162 CD1 LEU 834 **ATOM** 163 CD2 LEU 834 ATOM 164 C LEU 834 **ATOM** 165 O LEU 834 **ATOM** 166 N LYS 835 ATOM 168 CA LYS 835 ATOM 169 CB LYS 835 ATOM 170 CG LYS 835 **ATOM** 171 CD LYS 835 **ATOM** 172 CE LYS 835 ATOM 173 NZ LYS 835 ATOM 177 C LYS 835 ATOM 178 O LYS 835 ATOM 179 N LEU 836 ATOM 181 CA LEU 836 ATOM 182 CB LEU 836 ATOM 183 CG LEU 836 **ATOM** 184 CD1 LEU 836 **ATOM** 185 CD2 LEU 836 **ATOM** 186 C LEU 836 **ATOM** 187 O LEU 836 **ATOM** 188 N GLY 837 **ATOM** 190 CA GLY 837 ATOM: 191 C GLY 837 ATOM 192 O GLY 837 **ATOM** 193 N LYS 838 **ATOM** 195 CA LYS 838 **ATOM** 196 CB LYS 838 **ATOM** 197 C LYS 838 **ATOM** 198 O LYS 838 ATOM 199 N PRO 839 ATOM 200 CD PRO 839 ATOM 201 CA PRO 839 ATOM 202 CB PRO 839 . ATOM 203 CG PRO 839 ATOM 204 C PRO 839 ATOM 205 O PRO 839 ATOM 206 N LEU 840 ATOM

24.289 47.370 14.690 1.00 18.27 25.013 47.943 16.747 1.00 18.35 25.089 46.600 17.329 1.00 22.59 26.488 46.398 17.946 1.00 25.91 27.073 45.003 18.139 1.00 24.64 27.185 44.327 16.805 1.00 21.77 28.428 45.085 18.785 1.00 17.43 23.988 46.326 18.387 1.00 24.77 23.886 46.973 19.433 1.00 24.03 23.173 45.335 18.087 1.00 28.94 22.072 44.942 18.940 1.00 32.84 20.794 44.913 18.081 1.00 31.34 19.529 44.697 18.839 1.00 36.63 18.359 44.407 17.940 1.00 39.31 17.074 44.414 18.783 1.00 48.99 17.074 43.448 19.950 1.00 48.86 22.431 43.532 19.420 1.00 31.79 22.408 42.609 18.616 1.00 34.57 22.854 43.395 20.680 1.00 33.17 23.229 42.101 21.277 1.00 34.01 23.970 42.292 22.593 1.00 33.96 25.400 42.796 22.462 1.00 42.50 26.082 42.858 23.854 1.00 41.15 26.153 41.860 21.501 1.00 40.93 22.053 41.181 21.547 1.00 33.27 21.017 41.631 22.025 1.00 31.15 22.268 39.882 21.330 1.00 36.34 21.228 38.881 21.536 1.00 34.95 21.603 37.761 22.497 1.00 35.64 22.203 37.980 23.554 1.00 39.23 21.254 36.541 22.126 1.00 35.31 21.531 35.375 22.962 1.00 37.86 20.647 34.192 22.539 1.00 41.52 22.991 34.935 22.989 1.00 35.93 23.650 34.851 21.946 1.00 34.37 23.499 34.608 24.187 1.00 33.68 22.820 34.757 25.486 1.00 34.48 24.880 34.158 24.363 1.00 37.11 24.927 33.750 25.833 1.00 37.46 23.970 34.710 26.472 1.00 37.04 25.148 32.963 23.474 1.00 39.09 24.303 32.085 23.327 1.00 38.13 26.261 33.013 22.767 1.00 43.08

FIG. 7(5)

208 CA LEU 840 ATOM 209 CB LEU 840 ATOM 210 CG LEU 840 ATOM 211 CD1 LEU 840 ATOM 212 CD2 LEU 840 ATOM 213 C LEU 840 ATOM 214 O LEU 840 ATOM 215 N GLY 841 ATOM 217 CA GLY 841 ATOM 218 C GLY 841 ATOM 219 O GLY 841 ATOM 220 N ARG 842 ATOM 222 CA ARG 842 ATOM 223 CB ARG 842 ATOM 224 C ARG 842 ATOM 225 O ARG 842 ATOM 226 N GLY 843 ATOM 228 CA GLY 843 ATOM 229 C GLY 843 **ATOM** 230 O GLY 843 **ATOM** 231 N ALA 844 **ATOM** 233 CA ALA 844 **ATOM** 234 CB ALA 844 ATOM 235 C ALA 844 **ATOM** 236 O ALA 844 ATOM 237 N PHE 845 ATOM 239 CA PHE 845 ATOM 240 CB PHE 845 ATOM 241 C PHE 845 MOTA 242 O PHE 845 ATOM 243 N GLY 846 ATOM 245 CA GLY 846 ATOM 246 C GLY 846 ATOM 247 O GLY 846 ATOM 248 N GLN 847 **ATOM** 250 CA GLN 847 ATOM 251 CB GLN 847 ATOM 252 CG GLN 847 ATOM 253 CD GLN 847 **ATOM** 254 OE1 GLN 847 **ATOM** 255 NE2 GLN 847 **ATOM** 258 C GLN 847 **ATOM** 259 O GLN 847 ATOM

26.646 31.915 21.917 1.00 47.73 27.396 32.426 20.692 1.00 41.83 26.386 32.957 19.697 1.00 39.60 27.080 33.697 18.595 1.00 42.69 25.582 31.795 19.156 1.00 38.40 27.523 30.987 22.747 1.00 54.84 27.479 29.768 22.577 1.00 59.76 28.248 31.563 23.706 1.00 60.51 29.140 30.781 24.547 1.00 60.96 29.660 31.544 25.750 1.00 63.95 29.497 32.764 25.857 1.00 64.35 30.279 30.809 26.668 1.00 65.26 30.823 31.388 27.887 1.00 65.12 30.027 30.897 29.091 1.00 61.50 32.300 30.995 28.004 1.00 64.23 32.957 30.720 26.986 1.00 68.80 32.822 31.003 29.226 1.00 60.14 34.206 30.639 29.453 1:00 60.53 34.676 31.165 30.789 1.00 62.56 33.902 31.764 31.535 1.00 61.31 35.925 30.888 31.140 1.00 66.30 36.450 31.390 32.403 1.00 69.69 37.655 30.574 32.851 1.00 68.47 36.839 32.855 32.212 1.00 73.15 36.723 33.667 33.144 1.00 75.00 37.251 33.184 30.981 1.00 76.12 37.699 34.538 30.618 1.00 74.99 39.135 34.479 30.014 1.00 72.01 36.766 35.353 29.700 1.00 73.81 36.404 36.499 30.020 1.00 76.82 36.368 34.767 28.576 1.00 68.48 35.527 35.495 27.645 1.00 61.76 34.102 35.023 27.606 1.00 57.98 33.658 34.305 28.491 1.00 59.43 33.400 35.413 26.553 1.00 55.08 32.006 35.050 26.354 1.00 52.26 31.160 35.668 27.449 1.00 55.14 29.706 35.703 27.075 1.00 61.40 28.951 36.735 27.844 1.00 65.75 27.772 36.543 28.150 1.00 69.74 29.614 37.852 28.166 1.00 68.83 31.508 35.573 25.001 1.00 47.29 31.637 36.764 24.713 1.00 52.89

FIG. 7(6)

ATOM. 260 N VAL 848 262 CA VAL 848 ATOM 263 CB VAL 848 **ATOM** 264 CG1 VAL 848 ATOM 265 CG2 VAL 848 ATOM 266 C VAL 848 **ATOM** 267 O VAL 848 ATOM 268 N ILE 849 **ATOM** 270 CA ILE 849 ATOM 271 CB ILE 849 ATOM 272 CG2 ILE 849 ATOM 273 CG1 ILE 849 **ATOM** 274 CD1 ILE 849 **ATOM** 275 C ILE 849 ATOM 276 O ILE 849 ATOM 277 N GLU 850 ATOM 279 CA GLU 850 ATOM 280 CB GLU 850 ATOM 281 CG GLU 850 282 CD GLU 850 ATOM ATOM 283 OE1 GLU 850 **ATOM** 284 OE2 GLU 850 **ATOM** 285 C GLU 850 ATOM 286 O GLU 850 ATOM 287 N ALA 851 ATOM 289 CA ALA 851 ATOM 290 CB ALA 851 **ATOM** 291 C ALA 851 ATOM 292 O ALA 851 ATOM 293 N ASP 852 ATOM 295 CA ASP 852 ATOM 296 CB ASP 852 ATOM 297 CG ASP 852 ATOM 298 OD1 ASP 852 ATOM 299 OD2 ASP 852 ATOM 300 C ASP 852 ATOM 301 O ASP 852 ATOM 302 N ALA 853 ATOM 304 CA ALA 853 ATOM 305 CB ALA 853 **ATOM** 306 C ALA 853 ATOM 307 O ALA 853 ATOM 308 N PHE 854 ATOM

30.912 34.707 24.195 1.00 38.17 30.418 35.122 22.898 1.00 30.28 30.792 34.137 21.833 1.00 28.01 30.542 34.744 20.442 1.00 23.32 32.239 33.759 22.016 1.00 22.18 28.920 35.262 22.939 1.00 31.80 28.221 34.525 23.625 1.00 32.87 28.410 36.196 22.166 1.00 29.87 26.990 36.436 22.159 1.00 25.35 26.602 37.448 23.328 1.00 31.46 27.766 38.373 23.732 1.00 32.09 25.353 38.244 23.003 1.00 31.00 24.895 39.035 24.199 1.00 37.56 26.493 36.851 20.798 1.00 23.02 27.167 37.540 20.070 1.00 27.56 25.376 36.294 20.390 1.00 25.56 24.802 36.626 19.107 1.00 26.63 23.577 35.785 18.894 1.00 27.45 23.414 35.361 17.487 1.00 34.57 22.155 34.590 17.293 1.00 34.46 21.602 34.655 16.184 1.00 42.38 21.710 33.924 18.248 1.00 40.93 24.422 38.111 19.028 1.00 27.83 24.240 38.755 20.047 1.00 25.02 24.291 38.640 17.814 1.00 29.11 23.958 40.043 17.621 1.00 27.32 25.080 40.922 18.170 1.00 18.65 23.731 40.387 16.160 1.00 26.61 24.328 39.785 15.283 1.00 26.99 22.836 41.343 15.917 1.00 30.82 22.538 41.862 14.566 1.00 31.76 21.050 42.186 14.386 1.00 39.33 20.222 40.993 13.993 1.00 47.41 19.687 40.330 14.906 1.00 54.12 20.066 40.754 12.775 1.00 53.02 23.265 43.204 14.506 1.00 25.97 23.096 44.021 15.416 1.00 21.64 24.099 43.411 13.495 1.00 20.18 24.818 44.672 13.342 1.00 23.55 26.305 44.440 13.292 1.00 23.32 24.311 45.222 12.026 1.00 23.89 24.079 44.439 11.108 1.00 26.15 24.044 46.526 11.936 1.00 22.87

FIG. 7(7)

310 CA PHE 854 ATOM 311 CB PHE 854 ATOM 312 CG PHE 854 ATOM 313 CD1 PHE 854 ATOM 314 CD2 PHE 854 ATOM 315 CE1 PHE 854 ATOM 316 CE2 PHE 854 ATOM 317 CZ PHE 854 ATOM 318 C PHE 854 **ATOM** 319 O PHE 854 **ATOM** 320 N GLY 855 ATOM 322 CA GLY 855 **ATOM** 323 C GLY 855 **ATOM** 324 O GLY 855 ATOM 325 N ILE 856 ATOM 327 CA ILE 856 ATOM 328 CB ILE 856 ATOM 329 CG2 ILE 856 ATOM 330 CG1 ILE 856 **ATOM** 331 CD1 ILE 856 ATOM 332 C ILE 856 **ATOM** 333 O ILE 856 **ATOM** 334 N ASP 857 **ATOM** 336 CA ASP 857 ATOM 337 CB ASP 857 ATOM 338 CG ASP 857 **ATOM** 339 OD1 ASP 857 ATOM 340 OD2 ASP 857 ATOM 341 C ASP 857 ATOM 342 O ASP 857 ATOM 343 N LYS 858 ATOM 345 CA LYS 858 ATOM 346 CB LYS 858 **ATOM** 347 CG LYS 858 **ATOM** 348 CD LYS 858 **ATOM** 349 CE LYS 858 ATOM 350 NZ LYS 858 ATOM 354 C LYS 858 **ATOM** 355 O LYS 858 ATOM 356 N THR 859 ATOM 358 CA THR 859 ATOM 359 CB THR 859 ATOM ATOM 360 OG1 THR 859

23.529 47.059 10.680 1.00 16.46 22.487 48.135 10.901 1.00 23.71 22.020 48.758 9.643 1.00 27.62 22.476 50.011 9.266 1.00 28.26 21.205 48.052 8.771 1.00 31.56 22.136 50.549 8.025 1.00 30.16 20.856 48.592 7.512 1.00 34.04 21.328 49.838 7.145 1.00 28.32 24.618 47.569 9.794 1.00 14.10 25.493 48.299 10.209 1.00 17.34 24.556 47.163 8.553 1.00 17.45 25.559 47.571 7.604 1.00 18.50 26.988 47.318 8.020 1.00 22.65 27.806 48.193 7.777 1.00 26.82 27.332 46.150 8.580 1.00 23.51 28.740 45.886 8.983 1.00 24.11 28.868 44.692 9.980 1.00 27.72 28.535 43.370 9.259 1.00 29.88 30.282 44.663 10.608 1.00 23.26 30.371 44.079 12.034 1.00 21.70 29.704 45.665 7.805 1.00 24.83 30.918 45.721 7.950 1.00 28.37 29.145 45.460 6.626 1.00 27.69 29.926 45.248 5.420 1.00 31.23 29.566 43.891 4.838 1.00 34.80 4.811 1.00 40.03 28.074 43.658 27.328 44.597 4.448 1.00 43.33 27.641 42.549 5.200 1.00 46.87 29.654 46.323 4.370 1.00 32.81 29.721 46.040 3.183 1.00 38.59 29.299 47.529 4.813 1.00 34.74 28.987 48.690 3.946 1.00 34.64 30.061 48.947 2.889 1.00 31.38 31.462 48.964 3.418 1.00 34.36 31.605 49.890 4.603 1.00 39.41 33.005 49.791 5.228 1.00 39.87 34.059 50.089 4.218 1.00 39.89 27.629 48.709 3.254 1.00 32.27 27.249 49.737 2.724 1.00 35.02 26.891 47.607 3.258 1.00 32.20 25.597 47.610 2.600 1.00 30.11 25.355 46.332 1.785 1.00 30.38 25.365 45.187 2.641 1.00 32.29

FIG. 7(8)

362 CG2 THR 859 ATOM 363 C THR 859 ATOM 364 O THR 859 **ATOM** 365 N ALA 860 **ATOM** 367 CA ALA 860 **ATOM** 368 CB ALA 860 ATOM 369 C ALA 860 **ATOM** 370 O ALA 860 ATOM 371 N THR 861 **ATOM** 373 CA THR 861 **ATOM** 374 CB THR 861 ATOM 375 OG1 THR 861 MOTA 377 CG2 THR 861 **ATOM** 378 C THR 861 **ATOM** 379 O THR 861 **ATOM** 380 N CYS 862 **ATOM** 382 CA CYS 862 ATOM 383 CB CYS 862 **ATOM** 384 SG CYS 862 **ATOM** 385 C CYS 862 **ATOM** 386 O CYS 862 ATOM 387 N ARG 863 **ATOM** 389 CA ARG 863 **ATOM** 390 CB ARG 863 **ATOM** 391 CG ARG 863 ATOM 392 CD ARG 863 ATOM 393 NE ARG 863 **ATOM** 395 CZ ARG 863 **ATOM** 396 NH1 ARG 863 **ATOM** 399 NH2 ARG 863 ATOM 402 C ARG 863 **ATOM** 403 O ARG 863 **ATOM** 404 N THR 864 **ATOM** 406 CA THR 864 **ATOM** 407 CB THR 864 **ATOM** 408 OG1 THR 864 **ATOM** 410 CG2 THR 864 ATOM 411 C THR 864 ATOM 412 O THR 864 **ATOM** 413 N VAL 865 **ATOM** 415 CA VAL 865 **ATOM** 416 CB VAL 865 ATOM 417 CG1 VAL 865 **ATOM**

26.437 46.179 0.757 1.00 32.22 24.450 47.839 3.546 1.00 28.71 24.577 47.647 4.750 1.00 30.55 23.303 48.201 2.989 1.00 30.07 22.123 48.474 3.784 1.00 28.01 21.141 49.253 2.928 1.00 23.78 21.461 47.222 4.394 1.00 28.00 20.251 47.100 4.373 1.00 31.77 22.228 46.325 5.008 1.00 29.99 21.663 45.078 5.577 1.00 27.77 22.186 43.857 4.808 1.00 20.97 23.614 43.926 4.687 1.00 27.23 21.608 43.794 3.449 1.00 29.39 21.986 44.790 7.055 1.00 31.89 23.095 45.077 7.532 1.00 34.73 21.037 44.183 7.770 1.00 34.09 21.250 43.805 9.178 1.00 31.63 19.922 43.756 9.943 1.00 27.50 19.863 44.908 11.327 1.00 41.79 21.876 42.424 9.146 1.00 25.51 21.241 41.492 8.700 1.00 30.38 23.136 42.307 9.541 1.00 27.68 23.839 41.025 9.532 1.00 28.29 25.211 41.210 8.882 1.00 36.18 25.775 39.945 8.275 1.00 48.71 27.282 40.034 7.943 1.00 58.46 27.824 38.721 7.550 1.00 65.04 29.112 38.452 7.330 1.00 65.66 29.482 37.219 6.985 1.00 67.60 30.030 39.409 7.421 1.00 66.49 24.006 40.409 10.943 1.00 28.34 24.337 41.125 11.904 1.00 24.64 23.735 39.100 11.078 1.00 23.23 23.900 38.426 12.364 1.00 18.91 23.062 37.099 12.489 1.00 19.40 21.672 37.435 12.547 1.00 24.20 23.371 36.351 13.793 1.00 8.83 25.385 38.148 12.462 1.00 20.93 26:001 37.736 11.468 1.00 20.14 25.962 38.442 13.634 1.00 16.03 27.381 38.254 13.897 1.00 16.69 28.175 39.620 13.906 1.00 17.70 28.107 40.299 12.539 1.00 21.22 i.

FIG. 7(9)

ATOM 418 CG2 VAL 865 419 C VAL 865 **ATOM** 420 O VAL 865 ATOM 421 N ALA 866 ATOM 423 CA ALA 866 ATOM 424 CB ALA 866 ATOM 425 C ALA 866 **ATOM** 426 O ALA 866 ATOM 427 N VAL 867 ATOM 429 CA VAL 867 ATOM 430 CB VAL 867 **ATOM** 431 CG1 VAL 867 ATOM 432 CG2 VAL 867 **ATOM** 433 C VAL 867 **ATOM** 434 O VAL 867 ATOM 435 N LYS 868 ATOM 437 CA LYS 868 **ATOM** 438 CB LYS 868 ATOM 439 CG LYS 868 ATOM 440 CD LYS 868 ATOM 441 CE LYS 868 ATOM 442 NZ LYS 868 **ATOM** 446 C LYS 868 ATOM 447 O LYS 868 ATOM 448 N MET 869 ATOM 450 CA MET 869 **ATOM** 451 CB MET 869 ATOM 869 452 CG MET ATOM 453 SD MET 869 ATOM 454 CE MET 869 **ATOM** 455 C MET 869 ATOM 456 O MET 869 ATOM 457 N LEU 870 **ATOM** 459 CA LEU 870 **ATOM** 460 CB LEU 870 **ATOM** 461 CG LEU 870 **ATOM** 462 CD1 LEU 870. ATOM 463 CD2 LEU 870 **ATOM** 464 C LEU 870 ATOM 465 O LEU 870 ATOM 466 N LYS 871 ATOM 468 CA LYS 871 ATOM 469 CB LYS 871 ATOM

27.625 40.554 14.979 1.00 20.92 27.533 37.660 15.276 1.00 15.90 26.552 37.554 15.995 1.00 16.43 28.775 37.295 15.612 1.00 16.37 29.210 36.753 16.910 1.00 18.08 30.022 35.490 16.691 1.00 7.41 30.117 37.834 17.588 1.00 23.87 31.121 38.261 16.998 1.00 24.17 29.790 38.235 18.827 1.00 26.69 30.534 39.268 19.554 1.00 20.37 29.592 40.365 20.088 1.00 17.71 30.361 41.586 20.519 1.00 9.32 28.635 40.753 19.027 1.00 14.57 31.320 38.748 20.728 1.00 21.67 30.784 38.085 21.606 1.00 23.57 32.616 38.982 20.694 1.00 21.65 33.471 38.593 21.782 1.00 27.02 34.860 38.169 21.289 1.00 29.71 34.842 36.963 20.405 1.00 37.08 36.151 36.810 19.666 1.00 44.81 36.183 35.512 18.868 1.00 45.52 37.548 35.298 18.274 1.00 47.28 33.585 39.842 22.647 1.00 26.11 33.962 40.914 22.188 1.00 24.72 33.184 39.721 23.888 1.00 29.77 33.299 40.821 24.803 1.00 32.95 31.958 41.491 24.996 1.00 30.57 30.900 40.542 25.463 1.00 32.29 29.348 41.157 24.961 1.00 42.68 29.251 42.663 25.919 1.00 35.32 33.778 40.205 26.095 1.00 40.29 33.921 38.967 26.216 1.00 35.26 34.079 41.066 27.051 1.00 46.88 34.521 40.576 28.337 1.00 51.36 35.544 41.549 28.937 1.00 48.55 36.862 41.677 28.180 1.00 44.32 37.734 42.739 28.855 1.00 36.89 37.535 40.306 28.149 1.00 41.04 33.344 40.306 29.311 1.00 53.63 32.163 40.615 29.037 1.00 52.68 33.675 39.644 30.412 1.00 56.89 32.695 39.346 31.426 1.00 58.53 33.083 38.077 32.169 1.00 59.89

FIG. 7(10)

470 CG LYS 871 ATOM 471 CD LYS 871 **ATOM** 472 CE LYS 871 **ATOM** 473 NZ LYS 871 ATOM 477 C LYS 871 ATOM 478 O LYS 871 ATOM 479 N GLU 872 **ATOM** 481 CA GLU 872 **ATOM** 482 CB GLU 872 ATOM 483 CG GLU 872 **ATOM** 484 CD GLU 872 **ATOM** 485 OE1 GLU 872 **ATOM** 486 OE2 GLU 872 **ATOM** 487 C GLU 872 **ATOM** 488 O GLU 872 **ATOM** 489 N GLY 873 ATOM 491 CA GLY 873 **ATOM** 492 C GLY 873 **ATOM** 493 O GLY 873 ATOM 494 N ALA 874 **ATOM** 496 CA ALA 874 ATOM 497 CB ALA 874 **ATOM** 498 C ALA 874 ATOM 499 O ALA 874 **ATOM** 500 N THR 875 **ATOM** 502 CA THR 875 **ATOM** 503 CB THR 875 **ATOM** 504 OG1 THR 875 **ATOM** 506 CG2 THR 875 **ATOM** 507 C THR 875 **ATOM** 508 O THR 875 **ATOM** 509 N HIS 876 ATOM 511 CA HIS 876 **ATOM** 512 CB HIS 876 ATOM 513 CG HIS 876 **ATOM** 514 CD2 HIS 876 **ATOM** 515 ND1 HIS 876 ATOM 517 CE1 HIS 876 ATOM 518 NE2 HIS 876 ATOM 520 C HIS 876 ATOM 521 O HIS 876 **ATOM** 522 N SER 877 **ATOM** 524 CA SER 877 ATOM

31.903 37.220 32.546 1.00 63.81 31.912 35.965 31.719 1.00 65.43 33.268 35.318 31.853 1.00 70.59 33.318 34.051 31.135 1.00 76.57 32.649 40.518 32.404 1.00 59.44 33.582 41.342 32.464 1.00 56.75 31.566 40.571 33.177 1.00 61.50 31.357 41.618 34.177 1.00 64.12 29.928 41.539 34.739 1.00 66.85 28.846 41.903 33.729 1.00 71.27 29.060 41.218 32.387 1.00 74.41 28.900 39.980 32.326 1.00 76.27 29.443 41.903 31.411 1.00 74.20 32.387 41.424 35.288 1.00 60.87 32.331 40.441 36.026 1.00 61.34 33.368 42.319 35.335 1.00 57.40 34.408 42.223 36.337 1.00 53.93 35.703 41.641 35.803 1.00 52.30. 36.518 41.103 36.563 1.00 51.95 35.881 41.721 34.491 1.00 51.13 37.090 41.217 33.862 1.00 51.21 36.875 41.049 32.335 1.00 48.57 38.270 42.172 34.199 1.00 50.40 38.101 43.388 34.369 1.00 48.57 39.465 41.609 34.245 1.00 48.33 40.657 42.334 34.617 1.00 51.59 41.572 41.428 35.447 1.00 54.42 42.677 42.184 35.937 1.00 60.69 42.107 40.280 34.593 1.00 60.52 41.455 42.830 33.448 1.00 51.15 41.395 42.263 32.372 1.00 52.26 42.343 43.770 33.733 1.00 53.93 43.215 44.392 32.737 1.00 55.68 44.170 45.383 33.419 1.00 54.06 45.609 44.980 33.361 1.00 56.52 46.595 45.314 32.487 1.00 56.83 46.191 44.149 34.297 1.00 60.22 47.472 43.992 34.009 1.00 62.12 47.739 44.689 32.916 1.00 59.66 44.003 43.385 31.898 1.00 54.72 44.510 43.712 30.810 1.00 54.08 44.167 42.189 32.434 1.00 52.07 44.872 41.160 31.704 1.00 53.73

FIG. (11)

ATOM 525 CB SER 877 ATOM 526 OG SER 877 528 C SER 877 **ATOM** 529 O SER 877 **ATOM** 530 N GLU 878 **ATOM** 532 CA GLU 878 ATOM 533 CB GLU 878 **ATOM** 534 CG GLU 878 **ATOM** 535 CD GLU 878 **ATOM** 536 OE1 GLU 878 **ATOM** 537 OE2 GLU 878 **ATOM** 538 C GLU 878 ATOM 539 O GLU 878 **ATOM** 540 N HIS 879 ATOM 542 CA HIS 879 ATOM 543 CB HIS 879 ATOM 544 CG HIS 879 ATOM 545 CD2 HIS 879 ATOM 546 ND1 HIS 879 ATOM548 CE1 HIS 879 ATOM 549 NE2 HIS 879 ATOM 551 C HIS 879 ATOM 552 O HIS 879 **ATOM** 553 N ARG 880 ATOM 555 CA ARG 880 **ATOM** 556 CB ARG 880 ATOM 557 CG ARG 880 ATOM 558 CD ARG 880 ATOM 559 NE ARG 880 ATOM 561 CZ ARG 880 ATOM 562 NH1 ARG 880 ATOM 565 NH2 ARG 880 ATOM 568 C ARG 880 ATOM 569 O ARG 880 **ATOM** 570 N ALA 881 ATOM 572 CA ALA 881 ATOM 573 CB ALA 881 **ATOM** 574 C ALA 881 **ATOM** 575 O ALA 881 ATOM 576 N LEU 882 **ATOM** 578 CA LEU 882 **ATOM** 579 CB LEU 882 **ATOM** 580 CG LEU 882 ATOM

45.622 40.256 32.669 1.00 57.58 46.559 41.054 33.379 1.00 63.62 43.880 40.410 30.810 1.00 51.29 44.227 39.962 29.715 1.00 50.11 42.629 40.320 31.246 1.00 47.72 41.620 39.696 30.410 1.00 45.39 40.335 39.483 31.201 1.00 48.19 40.383 38.191 32.013 1.00 60.86 39.304 38.086 33.092 1.00 68.27 38.448 37.162 33.027 1.00 70.85 39.336 38.911 34.029 1.00 67.92 41.448 40.702 29.277 1.00 40.09 41.536 40.365 28.104 1.00 38.92 41.393 41.966 29.659 1.00 34.60 41.252 43.072 28.732 1.00 36.68 41.070 44.392 29.505 1.00 44.03 40.637 45.547 28.652 1.00 43.54 39.403 46.025 28.364 1.00 40.08 41.529 46.307 27.917 1.00 39.08 40.860 47.192 27.202 1.00 40.82 39.572 47.045 27.452 1.00 49.01 42.455 43.172 27.797 1.00 34.17 42.293 43.494 26.626 1.00 33.65 43.664 42.993 28.319 1.00 33.25 44.838 43.033 27.470 1.00 29.84 46.124 42.932 28.299 1.00 36.53 46.615 41.470 28.452 1.00 50.57 48.121 41.276 28.649 1.00 56.95 48.555 41.748 29.960 1.00 63.99 49.030 42.967 30.175 1.00 66.67 49.391 43.327 31.397 1.00 66.45 49.170 43.813 29.157 1.00 66.52 44.741 41.799 26.533 1.00 29.72 45.246 41.808 25.401 1.00 21.81 44.070 40.747 27.006 1.00 28.49 43.942 39.514 26.227 1.00 31.72 43.587 38.342 27.142 1.00 31.57 -42.978 39.592 25.044 1.00 29.98 43.319 39.154 23.944 1.00 31.95 41.766 40.099 25.273 1.00 27.12 40.804 40.248 24.193 1.00 27.43 39.493 40.784 24.728 1.00 23.93 38.402 40.925 23.662 1.00 25.91 FIG. (12)

581 CD1 LEU 882 ATOM ATOM 582 CD2 LEU 882 583 C LEU 882 **ATOM** 584 O LEU 882 **ATOM** 585 N MET 883 **ATOM** 587 CA MET 883 ATOM 588 CB MET 883 ATOM 589 CG MET 883 ATOM 590 SD MET 883 **ATOM** 591 CE MET 883 **ATOM** 592 C MET 883 ATOM 593 O MET 883 **ATOM** 594 N SER 884 **ATOM** 596 CA SER 884 **ATOM** 597 CB SER 884 **ATOM** 598 OG SER 884 ATOM 600 C SER 884 ATOM 601 O SER 884 ATOM 602 N GLU 885 **ATOM** 604 CA GLU 885 ATOM 605 CB GLU 885 **ATOM** 606 CG GLU 885 **ATOM** 607 CD GLU 885 **ATOM** 608 OE1 GLU 885 **ATOM** 609 OE2 GLU 885 **ATOM** 610 C GLU 885 **ATOM** 611 O GLU 885 **ATOM** 612 N LEU 886 **ATOM** 614 CA LEU 886 **ATOM** 615 CB LEU 886 **ATOM** 616 CG LEU 886 **ATOM** 617 CD1 LEU 886 ATOM 618 CD2 LEU 886 ATOM 619 C LEU 886 **ATOM** 620 O LEU 886 **ATOM** 621 N LYS 887 ATOM 623 CA LYS 887 ATOM 624 CB LYS 887 ATOM 625 CG LYS 887 **ATOM** 626 CD LYS 887 **ATOM** 627 CE LYS 887 **ATOM** 628 NZ LYS 887 ATOM 632 C LYS 887 ATOM

38.435 39.722 22.743 1.00 21.91 37.013 41.102 24.325 1.00 23.61 41.368 41.230 23.151 1.00 30.62 41.312 40.982 21.945 1.00 27.61 41.940 42.325 23.643 1.00 29.74 42.548 43.364 22.808 1.00 30.75 43.001 44.516 23.738 1.00 27.47 43.432 45.828 23.084 1.00 33.64 42.313 46.592 21.882 1.00 33.18 41.031 47.285 22.943 1.00 33.54 43.711 42.756 21.965 1.00 29.92 43.862 43.022 20.766 1.00 28.38 44.501 41.893 22.588 1.00 29.75 45.597 41.231 21.912 1.00 28.29 46.343 40.391 22.923 1.00 32.03 47.220 39.502 22.270 1.00 44.59 45.091 40.329 20.778 1.00 29.39 45.595 40.359 19.654 1.00 28.92 44.084 39.526 21.071 1.00 25.33 43.559 38.661 20.058 1.00 27.47 42.563 37.692 20.661 1.00 31.61 41.142 38.108 20.642 1.00 46.01 40.215 36.903 20.799 1.00 55.19 40.018 36.469 21.964 1.00 58.80 39.715 36.379 19.762 1.00 54.01 42.945 39.470 18.924 1.00 28.59 42.833 38.983 17.805 1.00 26.67 42.560 40.712 19.211 1.00 27.06 41.994 41.594 18.205 1.00 23.75 41.483 42.887 18.847 1.00 22.79 41.122 44.033 17.905 1.00 17.60 39.981 43.608 16.999 1.00 11.98 40.747 45.285 18.702 1.00 18.31 43.049 41.936 17.147 1.00 24.77 42.767 41.880 15.939 1.00 22.15 44.265 42.246 17.602 1.00 25.08 45.384 42.613 16.722 1.00 24.94 46.517 43.227 17.544 1.00 29.70 46.105 44.304 18.560 1.00 30.67 45.556 45.551 17.895 1.00 28.99 45.170 46.645 18.923 1.00 26.07 46.354 47.216 19.621 1.00 17.59 45.921 41.407 15.925 1.00 25.59

FIG. 7(13)

ATOM 633 O LYS 887 634 N ILE 888 ATOM 636 CA ILE 888 **MOTA** 637 CB ILE 888 ATOM 638 CG2 ILE 888 ATOM 639 CG1 ILE 888 ATOM 640 CD1 ILE 888 **MOTA** 641 C ILE 888 **ATOM** 642 O ILE 888 **ATOM** 643 N LEU 889 ATOM 645 CA LEU 889 ATOM 646 CB LEU 889 **ATOM** 647 CG LEU 889 **ATOM** 648 CD1 LEU 889 **ATOM** 649 CD2 LEU 889 ATOM 650 C LEU 889 ATOM 651 O LEU 889 **ATOM** 652 N ILE 890 **ATOM** 654 CA ILE 890 ATOM 655 CB ILE 890 ATOM 656 CG2 ILE 890 ATOM 657 CG1 ILE 890 ATOM 658 CD1 ILE 890 ATOM 659 C ILE 890 ATOM 660 O ILE 890 ATOM 661 N HIS 891 ATOM 663 CA HIS 891 ATOM 664 CB HIS 891 ATOM 665 CG HIS 891 ATOM 666 CD2 HIS 891 ATOM 667 ND1 HIS 891 ATOM 669 CE1 HIS 891 ATOM 670 NE2 HIS 891 **ATOM** 672 C HIS 891 ATOM 673 O HIS 891 ATOM 674 N ILE 892 ATOM 676 CA ILE 892 ATOM 677 CB ILE 892 ATOM 678 CG2 ILE 892 ATOM 679 CG1 ILE 892 ATOM 680 CD1 ILE 892 ATOM 681 C ILE 892 ATOM 682 O ILE 892 ATOM

46.388 41.547 14.793 1.00 30.23 45.917 40.235 16.542 1.00 20.48 46.347 39.028 15.859 1.00 21.46 46.306 37.795 16.816 1.00 22.73 46.604 36.556 16.047 1.00 24.05 47.355 37.929 17.937 1.00 23.32 47.092 37.058 19.190 1.00 18.29 45.392 38.822 14.663 1.00 19.51 45.834 38.710 13.529 1.00 19.15 44.088 38.828 14.922 1.00 15.54 43.078 38.677 13.872 1.00 20.73 41.658 38.818 14.446 1.00 19.41 41.204 37.652 15.372 1.00 22.61 39.735 37.752 15.697 1.00 13.49 41.500 36.263 14.764 1.00 18.87 43.308 39.678 12.762 1.00 24.12 43.342 39.344 11.584 1.00 28.65 43.461 40.931 13.138 1.00 29.62 43.753 41.953 12.158 1.00 26.41 43.966 43.310 12.865 1.00 24.45 44.555 44.333 11.888 1.00 30.36 42.645 43.825 13.438 1.00 19.80 42.812 45.061 14.241 1.0014.93 45.053 41.519 11.415 1.00 28.37 45.126 41.553 10.191 1.00 24.83 46.066 41.099 12.164 1.00 27.37 47.309 40.659 11.567 1.00 27.76 48.277 40.175 12.654 1.00 36.80 49.509 39.507 12.100 1.00 47.58 50.811 39.869 12.147 1.00 46.38 49.450 38.394 11.276 1.00 52.71 50.660 38.114 10.825 1.00 50.46 51.505 38.993 11.340 1.00 54.62 47.098 39.536 10.537 1.00 27.01 47.522 39.647 9.402 1.00 32.82 46.580 38.403 10.995 1.00 24.99 46.300 37.216 10.181 1.00 23.19 45.233 36.282 10.907 1.00 24.73 44.643 35.295 9.941 1.00 20.03 45.828 35.522 12.104 1.00 26.32 47.015 36.222 12.787 1.00 36.72 45.700 37.625 8.848 1.00 22.57 46.115 37.155 7.775 1.00 25.20

FIG. 7(14)

683 N GLY 893 ATOM 685 CA GLY 893 **ATOM** 686 C GLY 893 ATOM 687 O GLY 893 **ATOM** 688 N HIS 894 **ATOM** 690 CA HIS 894 MOTA 691 CB HIS 894 **ATOM** 692 CG HIS 894 **ATOM** 693 CD2 HIS 894 **ATOM** 694 ND1 HIS 894 **ATOM** 696 CE1 HIS 894 **ATOM** 697 NE2 HIS 894 ATOM 699 C HIS 894 ATOM 700 O HIS 894 ATOM 701 N HIS 895 ATOM 703 CA HIS 895 ATOM 704 CB HIS 895 ATOM 705 CG HIS 895 ATOM 706 CD2 HIS 895 **ATOM** 707 ND1 HIS 895 ATOM 709 CE1 HIS 895 **ATOM** 710 NE2 HIS 895 **ATOM** 712 C HIS 895 **ATOM** 713 O HIS 895 **ATOM** 714 N LEU 896 ATOM 716 CA LEU 896 ATOM 717 CB LEU 896 **ATOM** 718 CG LEU 896 **ATOM** 719 CD1 LEU 896 **ATOM** 720 CD2 LEU 896 **ATOM** 721 C LEU 896 ATOM 722 O LEU 896 **ATOM** 723 N ASN 897 **ATOM** 725 CA ASN 897 **ATOM** 726 CB ASN 897 **ATOM** 727 CG ASN 897 **ATOM** 728 OD1 ASN 897 **ATOM** 729 ND2 ASN 897 ATOM 732 C ASN 897 ATOM 733 O ASN 897 **ATOM** 734 N VAL 898 **ATOM** 736 CA VAL 898 **ATOM** 737 CB VAL 898 **ATOM**

44.699 38.492 8.916 1.00 23.88 44.034 38.910 7.702 1.00 25.37 42.794 38.080 7.403 1.00 25.54 42.303 37.326 8.224 1.00 32.60 42.327 38.149 6.176 1.00 26.97 41.120 37.457 5.797 1.00 26.35 40.233 38.464 5.042 1.00 31.72 39.114 37.833 4.274 1.00 35.68 4.608 1.00 34.18 37.818 37.609 2.989 1.00 38.36 39.271 37.346 38.121 36.854 2.568 1.00 36.24 37.224 37.004 3.527 1.00 35.86 4.958 1.00 24.38 41.253 36.182 42.045 36.108 4.007 1.00 24.24 40.426 35.202 5.280 1.00 17.00 40.379 33.994 4.494 1.00 18.62 41.363 32.929 4.931 1.00 15.85 41.446 31.814 3.943 1.00 21.47 42.076 31.737 2.745 1.00 17.93 40.675.30.676 4.042 1.00 21.96 40.819 29.956 2.938 1.00 21.22 41.663 30.578 2.137 1.00 10.16 38.979 33.467 4.626 1.00 15.66 38.396 33.656 5.663 1.00 18.76 38.419 32.865 3.567 1.00 21.74 37.042 32.306 3.584 1.00 18.37 36.652 31.762 2.210 1.00 17.64 35.297 31.068 2.218 1.00 25.15 34.218 32.077 2.454 1.00 24.41 35.042 30.342 0.934 1.00 25.59 36.867 31.172 4.569 1.00 17.58 35.783 30.937 5.068 1.00 23.11 4.849 1.00 15.99 37.952 30.475 37.878 29.340 5.725 1.00 18.36 5.078 1.00 20.86 38.589 28.134 3.747 1.00 16.88 37.928 27.689 38.567 27.692 2.694 1.00 14.51 3.799 1.00 12.11 36.639 27.346 38.293 29.541 7.188 1.00 25.65 7.858 1.00 22.22 38.648 28.556 38.357 30.800 7.660 1.00 23.53 38.631 31.079 9.081 1.00 15.38 40.036 31.719 9.457 1.00 11.47

FIG. 7(15)

738 CG1 VAL 898 ATOM 739 CG2 VAL 898 **ATOM** 740 C VAL 898 **ATOM** 741 O VAL 898 ATOM 742 N VAL 899 ATOM 744 CA VAL 899 ATOM 745 CB VAL 899 **ATOM** 746 CG1 VAL 899 **ATOM** 747 CG2 VAL 899 **ATOM** 748 C VAL 899 **ATOM** 749 O VAL 899 ATOM 750 N ASN 900 **ATOM** 752 CA ASN 900 **ATOM** 753 CB ASN 900 **ATOM** 754 CG ASN 900 ATOM 755 OD1 ASN 900 ATOM 756 ND2 ASN 900 **ATOM** 759 C ASN 900 **ATOM** 760 O ASN 900 **ATOM** 761 N LEU 901 **ATOM** 763 CA LEU 901 **ATOM** 764 CB LEU 901 **ATOM** 765 CG LEU 901 **ATOM** 766 CD1 LEU 901 **ATOM** 767 CD2 LEU 901 **ATOM** 768 C LEU 901 **ATOM** 769 O LEU 901 **ATOM** 770 N LEU 902 **ATOM** 772 CA LEU 902 ATOM 773 CB LEU 902 **ATOM** 774 CG LEU 902 **ATOM** 775 CD1 LEU 902 **ATOM** 776 CD2 LEU 902 ATOM 777 C LEU 902 ATOM 778 O LEU 902 **ATOM** 779 N GLY 903 **ATOM** 781 CA GLY 903 **ATOM** 782 C GLY 903 **ATOM** 783 O GLY 903 **ATOM** 784 N ALA 904 **ATOM** 786 CA ALA 904 **ATOM** 787 CB ALA 904 **ATOM** 788 C ALA 904 ATOM

41.146 30.813 9.017 1.00 14.76 40.236 33.119 8.883 1.00 8.71 37.475 31.959 9.477 1.00 15.57 36.698 32.382 8.620 1.00 17.87 37.226 32.049 10.773 1.00 18.55 36.155 32.882 11.264 1.00 20.68 35.757 32.487 12.720 1.00 19.98 34.618 33.384 13.202 1.00 18.29 35.346 31.016 12.788 1.00 12.67 36.807 34.272 11.244 1.00 21.95 37.725 34.517 12.003 1.00 21.42 36.352 35.164 10.363 1.00 23.43 36.930 36.526 10.226 1.00 23.52 36.737 37.061 8.803 1.00 19.45 37.350 36.177 7.782 1.00 19.58 38.578 36.087 7.667 1.00 17.65 36.511 35.528 7.004 1.00 20.34 36.484 37.641 11.152 1.00 17.00 35.343 37.704 11.598 1.00 16.94 37.413 38.544 11.384 1.00 17.25 37.167-39.733 12.160 1.00 17.98 38.494 40.447 12.426 1.00 16.80 38.444 41.819 13.101 1.00 14.17 38.018 41.673 14.560 1.00 11.71 39.782 42.435 13.008 1.00 2.76 36.354 40.578 11.174 1.00 20.28 36.669 40.612 9.965 1.00 18.06 35.280 41.180 11.686 1.00 19.74 34.398 42.031 10.917 1.00 15.84 32.950 41.593 11.087 1.00 11.70 32.615 40.230 10.473 1.00 13.49 31.142 39.827 10.774 1.00 13.78 32.856 40.270 8.981 1.00 12.15 34.566 43.486 11.345 1.00 19.59 34.466 44.380 10.510 1.00 23.95 34.854 43.724 12.625 1.00 20.15 35.037 45.090 13.114 1.00 21.60 35.147 45.075 14.620 1.00 24.02 35.070 43.991 15.194 1.00 26.53 35.305 46.236 15.269 1.00 25.19 35.411 46.293 16.740 1.00 18.80 36.830 46.074 17.177 1.00 12.62 34.886 47.559 17.386 1.00 20.83

FIG. 7(16)

ATOM 789 O ALA 904 790 N CYS 905 **ATOM** 792 CA CYS 905 **ATOM** 793 CB CYS 905 **ATOM** 794 SG CYS 905 **ATOM** 795 C CYS 905 **ATOM** 796 O CYS 905 **ATOM** 797 N THR 906 **ATOM** 799 CA THR 906 **ATOM** 800 CB THR 906 **ATOM** 801 OG1 THR 906 **ATOM** 803 CG2 THR 906 **ATOM** 804 C THR 906 **ATOM** 805 O THR 906 **ATOM** 806 N LYS 907 **ATOM** 808 CA LYS 907 **ATOM** 809 CB LYS 907 **ATOM** 810 CG LYS 907 ATOM 811 CD LYS 907 ATOM 812 CE LYS 907 **ATOM** 813 NZ LYS 907 **ATOM** 817 C LYS 907 **ATOM** 818 O LYS 907 **ATOM** 819 N PRO 908 **ATOM** 820 CD PRO 908 **ATOM** 821 CA PRO 908 **ATOM** 822 CB PRO 908 ATOM 823 CG PRO 908 **ATOM** 824 C PRO 908 **ATOM** 825 O PRO 908 **ATOM** 826 N GLY 909 ATOM 828 CA GLY 909 **ATOM** 829 C GLY 909 **ATOM** 830 O GLY 909 ATOM 831 N GLY 910 ATOM 833 CA GLY 910 **ATOM** 834 C GLY 910 ATOM 835 O GLY 910 **ATOM** 836 N PRO 911 ATOM 837 CD PRO 911 **ATOM** 838 CA PRO 911 **ATOM** 839 CB PRO 911 ATOM 840 CG PRO 911 MOTA

34.789 48,616 16.765 1.00 26.12 34.617 47.443 18.674 1.00 21.21 34.128 48.530 19.493 1.00 19.91 32.804 48.160 20.115 1.00 16.08 31.561 47.894 18.851 1.00 15.32 35.176 48.687 20.556 1.00 23.00 35.245 47.890 21.486 1.00 24.21 36.042 49.674 20.361 1.00 26.02 37.140 49.945 21.283 1.00 29.46 38.514 49.768 20.574 1.00 26.67 38.635 50.739 19.526 1.00 29.06 38.648 48.363 20.001 1.00 23.13 37.130 51.346 21.928 1.00 30.07 37.642 51.522 23.036 1.00 29.29 36.582 52.332 21.228 1.00 32.81 36.554 53.686 21.745 1.00 39.38 35.982 54.637 20.701 1.00 41.03 34.536 54.432 20.386 1.00 48.86 34.071 55.528 19.427 1.00 57.25 33.996 56.878 20.143 1.00 63.62 33.688 58.001 19.213 1.00 68.81 35.796 53.779 23.070 1.00 44.43 35.094 52.867 23.442 1.00 44.52 36.034 54.838 23.857 1.00 49.18 37.147 55.794 23.712 1.00 50.93 35.358 55.022 25.149 1.00 46.86 35.963 56.324 25.647 1.00 49.68 37.387 56.216 25.143 1.00 51.43 33.852 55.145 25.036 1.00 44.06 33.345 55.600 24.008 1.00 44.40 33.154 54.772 26.110 1.00 41.44 31.698 54.842 26.135 1.00 37.38 30.999 53.502 26.035 1.00 38.26 29.778 53.439 25.751 1.00 40.07 31.753 52.424 26.264 1.00 36.39 31.178 51.087 26.190 1.00 34.35 32.180 49.961 26.360 1.00 31.85 33.394 50.235 26.528 1.00 27.95 31.710 48.686 26.319 1.00 27.95 30.280 48.339 26.197 1.00 28.51 32.511 47.463 26.467 1.00 25.21 31.438 46.393 26.724 1.00 27.44 30.315 46.840 25.891 1.00 22.45

FIG. 7(97)

841 C PRO 911 **ATOM** 842 O PRO 911 ATOM 843 N LEU 912 ATOM 845 CA LEU 912 ATOM 846 CB LEU 912 **MOTA** 847 CG LEU 912 ATOM 848 CD1 LEU 912 ATOM 849 CD2 LEU 912 ATOM 850 C LEU 912 ATOM 851 O LEU 912 ATOM 852 N MET 913 ATOM 854 CA MET 913 ATOM 855 CB MET 913 ATOM 856 CG MET 913 **ATOM** 857 SD MET 913 ATOM 858 CE MET 913 ATOM 859 C MET 913 ATOM 860 O MET 913 ATOM 861 N VAL 914 ATOM 863 CA VAL 914 ATOM 864 CB VAL 914 ATOM 865 CG1 VAL 914 ATOM 866 CG2 VAL 914 ATOM 867 C VAL 914 ATOM 868 O VAL 914 ATOM 869 N ILE 915 ATOM 871 CA ILE 915 ATOM 872 CB ILE 915 ATOM 873 CG2 ILE 915 ATOM 874 CG1 ILE 915 **MOTA** 875 CD1 ILE 915 ATOM 876 C ILE 915 ATOM 877 O ILE 915 ATOM 878 N VAL 916 ATOM 880 CA VAL 916 ATOM 881 CB VAL 916 ATOM 882 CG1 VAL 916 ATOM 883 CG2 VAL 916 ATOM 884 C VAL 916 ATOM 885 O VAL 916 ATOM 886 N GLU 917 ATOM 888 CA GLU 917 ATOM 889 CB GLU 917 ATOM

33.340 47.118 25.234 1.00 22.33 32.903 47.366 24.124 1.00 23.57 34.548 46.581 25.430 1.00 22.75 35.412 46.177 24.308 1.00 23.22 36.778 45.685 24.812 1.00 23.67 38.095 45.759 24.005 1.00 24.34 38.988 44.618 24.490 1.00 20.11 37.906 45.745 22.477 1.00 12.72 34.692 45.010 23.627 1.00 22.56 34.342 44.029 24.283 1.00 17.69 34.417 45.142 22.334 1.00 24.19 33.724 44.085 21.617 1.00 21.51 32.264 44.456 21.429 1.00 22.09 31.489 44.461 22.728 1.00 22.26 29.829 45.009 22.484 1.00 24.17 30.127 46.676 22.205 1.00 20.40 34.386 43.768 20.295 1.00 20.42 34.701 44.657 19.519 1.00 21.08 34.703 42.491 20.102 1.00 23.72 35.354 42.001 18.891 1.00 20.24 36.614 41.170 19.232 1.00 16.92 37.254 40.637 17.958 1.00 19.36 37.629 42.055 19.972 1.00 13.30 34.296 41.210 18.132 1.00 19.70 33.836 40.191 18.587 1.00 26.45 33.844 41.775 17.026 1.00 19.86 32.806 41.212 16.179 1.00 20.42 32.034 42.384 15.455 1.00 18.44 30.721 41.909 14.869 1.00 12.35 31.756 43.531 16.426 1.00 17.60 31.358 44.822 15.735 1.00 15.14 33.457 40.287 15.115 1.00 23.98 34.361 40.722 14.373 1.00 23.30 33.054 39.011 15.075 1.00 20.08 33.594 38.089 14.077 1.00 17.64 34.543 37.003 14.680 1.00 9.09 35.703 37.685 15.350 1.00 5.05 33.817 36.126 15.678 1.00 10.26 32.422 37.486 13.342 1.00 17.74 31.275 37.790 13.664 1.00 20.02 32.684 36.702 12.303 1.00 14.74 31.589 36.073 11.577 1.00 13.03 32.120 35.409 10.332 1.00 14.06

FIG. 7(8)

890 CG GLU 917 MOTA 891 CD GLU 917 ATOM 892 OE1 GLU 917 ATOM 893 OE2 GLU 917 **ATOM** 894 C GLU 917 ATOM 895 O GLU 917 ATOM 896 N PHE 918 ATOM 898 CA PHE 918 ATOM 899 CB PHE 918 ATOM 900 CG PHE 918 ATOM 901 CD1 PHE 918 **ATOM** 902 CD2 PHE 918 ATOM 903 CE1 PHE 918 **ATOM** 904 CE2 PHE 918 **ATOM** 905 CZ PHE 918 ATOM 906 C PHE 918 **ATOM** 907 O PHE 918 ATOM 908 N CYS 919 ATOM 910 CA CYS 919 **ATOM** 911 CB CYS 919 **ATOM** 912 SG CYS 919 **ATOM** 913 C CYS 919 **ATOM** 914 O CYS 919 **ATOM** 915 N LYS 920 **ATOM** 917 CA LYS 920 **ATOM** 918 CB LYS 920 ATOM 919 CG LYS 920 **ATOM** 920 CD LYS 920 **ATOM** 921 CE LYS 920 **ATOM** 922 NZ LYS 920 **ATOM** 926 C LYS 920 \boldsymbol{ATOM} 927 O LYS 920 **ATOM** 928 N PHE 921 **ATOM** 930 CA PHE 921 ATOM 931 CB PHE 921 **ATOM** 932 CG PHE 921 **ATOM** 933 CD1 PHE 921 ATOM 934 CD2 PHE 921 ATOM 935 CE1 PHE 921 **ATOM** 936 CE2 PHE 921 ATOM 937 CZ PHE 921 ATOM 938 C PHE 921 **ATOM** 939 O PHE 921 ATOM

32.946 36.348 9.464 1.00 24.11 33.543 35.651 8.258 1.00 26.52 33.060 35.904 7.139 1.00 27.67 34.480 34.841 8.425 1.00 28.39 30.853 35.051 12.434 1.00 14.78 31.445 34.344 13.234 1.00 14.35 29.557 34.958 12.229 1.00 19.12 28.688 34.042 12.966 1.00 18.07 27.334 34.721 13.168 1.00 18.48 26.275 33.840 13.748 1.00 17.83 26.328 33.456 15.081 1.00 18.65 25.213 33.400 12.953 1.00 21.10 25.336 32.639 15.613 1.00 18.12 24.210 32.580 13.473 1.00 14.29 24.274 32.201 14.799 1.00 17.78 28.487 32.805 12.113 1.00 18.83 28.081 32.917 10.964 1.00 11.61 28.761 31.635 12.676 1.00 19.49 28.590 30.372 11.947 1.00 19.00 29.855 29.566 12.069 1.00 16.78 31.225 30.428 11.325 1.00 16.84 27.383 29.659 12.556 1.00 21.18 27.474 29.135 13.676 1.00 20.69 26.269 29.653 11.818 1.00 18.06 24.998 29.130 12.318 1.00 28.13 23.799 29.581 11.459 1.00 25.17 23.595 28.799 10.207 1.00 33.78 22.658 29.509 9.250 1.00 40.32 21.261 29.706 9.829 1.00 51.94 20.343 30.396 8.845 1.00 56.09 24.813 27.679 12.700 1.00 28.53 24.020 27.405 13.592 1.00 31.57 25.533 26.757 12.078 1.00 24.89 25.328 25.362 12.409 1.00 21.12 25.497 24.518 11.171 1.00 20.75 24.588 24.917 10.084 1.00 22.95 23.224 24.734 10.219 1.00 27.55 25.077 25.564 8.975 1.00 29.40 22.362 25.205 9.269 1.00 35.42 24.237 26.041 8.013 1.00 32.24 22.869 25.870 8.154 1.00 38.81 26.158 24.823 13.535 1.00 21.23 26.002 23.664 13.900 1.00 22.74

FIG. 7(19)

940 N GLY 922 ATOM 942 CA GLY 922 **ATOM** 943 C GLY 922 **ATOM** 944 O GLY 922 ATOM 945 N ASN 923 ATOM 947 CA ASN 923 ATOM 948 CB ASN 923 **ATOM** 949 CG ASN 923 **ATOM** 950 OD1 ASN 923 **ATOM** 951 ND2 ASN 923 **ATOM** 954 C ASN 923 **ATOM** 955 O ASN 923 **ATOM** 956 N LEU 924 **ATOM** 958 CA LEU 924 **ATOM** 959 CB LEU 924 **ATOM** 960 CG LEU 924 **ATOM** 961 CD1 LEU 924 ATOM. 962 CD2 LEU 924 **ATOM** 963 C LEU 924 ATOM 964 O LEU 924 ATOM 965 N SER 925 ATOM 967 CA SER 925 **ATOM** 968 CB SER 925 **ATOM** 969 OG SER 925 **ATOM** 971 C SER 925 **ATOM** 972 O SER 925 ATOM 973 N THR 926 **ATOM** 975 CA THR 926 ATOM 976 CB THR 926 ATOM 977 OG1 THR 926 **ATOM** 979 CG2 THR 926 ATOM 980 C THR 926 **ATOM** 981 O THR 926 **ATOM** 982 N TYR 927 ATOM 984 CA TYR 927 ATOM 985 CB TYR 927 ATOM 986 CG TYR 927 ATOM 987 CD1 TYR 927 ATOM 988 CE1 TYR 927 ATOM 989 CD2 TYR 927 ATOM 990 CE2 TYR 927 ATOM 991 CZ TYR 927 ATOM 992 OH TYR 927 MOTA

27.047 25.659 14.065 1.00 18.39 27.906 25.257 15.172 1.00 17.62 29.115 24.455 14.759 1.00 18.42 29.331 24.230 13.581 1.00 20.81 29.903 24.011 15.729 1.00 22.93 31.092 23.223 15.430 1.00 24.85 31.867 22.837 16.705 1.00 29.68 31.212 21.710 17.493 1.00 39.14 31.252 20.550 17.087 1.00 41.11 30.662 22.038 18.660 1.00 35.87 30.818 22.019 14.523 1.00 21.09 29.685 21.566 14.370 1.00 20.59 31.867 21.523 13.896 1.00 21.13 31.740 20.431 12.957 1.00 22.85 33.019 20.377 12.126 1.00 23.67 33.019 19.462 10.920 1.00 17.22 31.776 19.699 10.125 1.00 18.21 34.268 19.729 10.095 1.00 23.82 31.414 19.062 13.558 1.00 22.65 30.601 18.326 13.013 1.00 26.13 31.035 18.742 14.687 1.00 20.06 31.853 17.463 15.383 1.00 25.99 32.741 17.400 16.623 1.00 27.28 32.426 16.272 17.416 1.00 32.86 30.432 17.217 15.812 1.00 26.73 29.863 16.148 15.552 1.00 30.93 29.892 18.190 16.534 1.00 24.48 28.535 18.129 16.996 1.00 19.27 28.258 19.336 17.901 1.00 16.05 29.230 19.374 18.951 1.00 18.42 26.927 19.216 18.550 1.00 13.93 27.610 18.048 15.758 1.00 20.47 26.654 17.258 15.711 1.00 25.12 27.961 18.760 14.701 1.00 18.97 27.128 18.715 13.515 1.00 20.97 27.597 19.720 12.464 1.00 18.52 26.708 19.683 11.230 1.00 18.69 25.391 20.196 11.266 1.00 14.64 24.567 20.173 10.125 1.00 13.73 27.173 19.138 10.031 1.00 22.28 26.347 19.104 8.879 1.00 24.92 25.058 19.626 8.944 1.00 16.40 24.285 19.600 7.819 1.00 23.87

FIG. 7(20)

ATOM 994 C TYR 927 995 O TYR 927 **ATOM** ATOM 996 N LEU 928 ATOM 998 CA LEU 928 ATOM 999 CB LEU 928 ATOM 1000 CG LEU 928 ATOM 1001 CD1 LEU 928 ATOM 1002 CD2 LEU 928 ATOM 1003 C LEU 928 ATOM 1004 O LEU 928 ATOM 1005 N ARG 929 ATOM 1007 CA ARG 929 ATOM 1008 CB ARG 929 ATOM 1009 CG ARG 929 ATOM 1010 CD ARG 929 ATOM 1011 NE ARG 929 ATOM 1013 CZ ARG 929 ATOM 1014 NH1 ARG 929 ATOM 1017 NH2 ARG 929 ATOM 1020 C ARG 929 ATOM 1021 O ARG 929 ATOM 1022 N SER 930 ATOM 1024 CA SER 930 ATOM 1025 CB SER 930 ATOM 1026 OG SER 930 ATOM 1028 C SER 930 ATOM 1029 O SER 930 ATOM 1030 N LYS 931 ATOM 1032 CA LYS 931 ATOM 1033 CB LYS 931 ATOM 1034 CG LYS 931 ATOM 1035 CD LYS 931 ATOM 1036 CE LYS 931 ATOM 1037 NZ LYS 931 ATOM 1041 C LYS 931 ATOM 1042 O LYS 931 ATOM 1043 N ARG 932 ATOM 1045 CA ARG 932 ATOM 1046 CB ARG 932 ATOM 1047 CG ARG 932 ATOM 1048 CD ARG 932 ATOM 1049 NE ARG 932 ATOM 1051 CZ ARG 932

27.118 17.343 12.855 1.00 23.85 26.078 16.860 12.428 1.00 24.11 28.313 16.793 12.665 1.00 28.91 28.513 15.495 12.020 1.00 31.09 30.017 15.192 11.863 1.00 27.50 30.813 16.159 10.953 1.00 24.21 32.302 15.880 11.065 1.00 24.38 30.343 16.097 9.514 1.00 12.63 27.801 14.369 12.747 1.00 31.00 27.164 13.540 12.117 1.00 31.53 27.883 14.351 14.067 1.00 34.05 27.193 13.316 14.833 1.00 40.50 27.406 13.552 16.325 1.00 41.71 28.358 12.605 16.969 1.00 40.42 29.253 13.359 17.908 1.00 49.36 28.521 13.947 19.020 1.00 62.28 28.946 14.985 19.749 1.00 65.86 28.178 15.432 20.753 1.00 66.98 30.122 15.573 19.492 1.00 58.39 25.678 13.304 14.529 1.00 42.76 25.075 12.234 14.370 1.00 44.84 25.089 14.498 14.412 1.00 41.42 23.663 14.677 14.150 1.00 37.04 23.324 16.151 14.250 1.00 38.80 23.662 16.816 13.041 1.00 37.58 23.226 14.226 12.774 1.00 38.41 22.034 14.254 12.451 1.00 43.98 24.179 13.865 11.936 1.00 37.60 23.845 13.472 10.590 1.00 38.82 24.575 14.387 9.606 1.00 43.10 24.388 15.864 9.884 1.00 45.62 22.999 16.302 9.487 1.00 49.49 22.901 16.444 7.985 1.00 46.94 21.501 16.690 7.568 1.00 49.54 24.136 12.011 10.264 1.00 39.02 23.991 11.615 9.111 1.00 42.79 24.522 11.199 11.247 1.00 37.44 24.793 9.776 10.971 1.00 38.33 25.149 9.020 12.244 1.00 33.55 26.456 9.461 12.798 1.00 33.92 26.812 8.729 14.043 1.00 35.88 28.223 8.929 14.368 1.00 43.26 28.720 8.909 15.604 1.00 45.56

FIG. 7(21)

ATOM 1052 NH1 ARG 932 ATOM 1055 NH2 ARG 932 ATOM 1058 C ARG 932 ATOM 1059 O ARG 932 ATOM 1060 N ASN 933 ATOM 1062 CA ASN 933 ATOM 1063 CB ASN 933 ATOM 1064 CG ASN 933 ATOM 1065 OD1 ASN 933 ATOM 1066 ND2 ASN 933 ATOM 1069 C ASN 933 ATOM 1070 O ASN 933 ATOM 1071 N GLU 934 ATOM 1073 CA GLU 934 ATOM 1074 CB GLU 934 ATOM 1075 CG GLU 934 ATOM 1076 CD GLU 934 ATOM 1077 OE1 GLU 934 ATOM 1078 OE2 GLU 934 ATOM 1079 C GLU 934 ATOM 1080 O GLU 934 ATOM 1081 N PHE 935 ATOM 1083 CA PHE 935 ATOM 1084 CB PHE 935 ATOM 1085 CG PHE 935 ATOM 1086 CD1 PHE 935 ATOM 1087 CD2 PHE 935 ATOM 1088 CE1 PHE 935 ATOM 1089 CE2 PHE 935 ATOM 1090 CZ PHE 935 ATOM 1091 C PHE 935 ATOM 1092 O PHE 935 ATOM 1093 N VAL 936 ATOM 1095 CA VAL 936 ATOM 1096 CB VAL 936 ATOM 1097 CG1 VAL 936 ATOM 1098 CG2 VAL 936 ATOM 1099 C VAL 936 ATOM 1100 O VAL 936 ATOM 1101 N PRO 937 ATOM 1102 CD PRO 937 ATOM 1103 CA PRO 937 ATOM 1104 CB PRO 937

30.018 9.098 15.809 1.00 47.32 27.916 8.725 16.645 1.00 53.04 23.621 9.087 10.273 1.00 41.54 23.821 8.135 9.532 1.00 41.31 22.412 9.582 10.536 1.00 44.37 21.181 9.069 9.956 1.00 47.14 19.974 9.453 10.824 1.00 54.55 19.783 8.545 12.050 1.00 57.14 20.622 7.693 12.369 1.00 54.11 18.668 8.752 12.757 1.00 57.76 20.974 9.680 8.589 1.00 49.60 20.260 9.125 7.753 1.00 55.62 21.494 10.888 8.403 1.00 52.11 21.365 11.580 7.122 1.00 52.39 20.859 13.007 7.323 1.00 56.14 19.434 13.095 7.822 1.00 59.40 19.332 13.686 9.211 1.00 63.97 18.427 13.250 9.953 1.00 69.17 20.138 14.580 9.563 1.00 64.27 22.677 11.593 6.332 1.00 50.45 23.188 12.663 5.961 1.00 50.70 23.205 10.396 6.070 1.00 46.25 24.440 10.225 5.325 1.00 41.20 25.638 10.121 6.268 1.00 40.97 26.923 9.800 5.555 1.00 39.81 27.327 8.478 5.378 1.00 34.65 27.676 10.815 4.970 1.00 33.02 28.455 8.180 4.617 1.00 32.30 28.793 10.515 4.218 1.00 29.96 29.181 9.201 4.037 1.00 29.08 24.474 9.006 4.412 1.00 40.49 24.394 7.871 4.865 1.00 40.47 24.694 9.237 3.133 1.00 38.66 24.809 8.138 2.208 1.00 43.29 23.663 8.113 1.221 1.00 40.39 23.739 9.312 0.280 1.00 34.50 23.720 6.841 0.444 1.00 42.47 26.087 8.436 1.438 1.00 49.63 26.322 9.585 1.081 1.00 55.64 26.960 7.433 1.222 1.00 50.29 26.966 6.087 1.822 1.00 49.69 28.207 7.669 0.483 1.00 50.65 28.676 6.260 0.177 1.00 46.68

FIG. 7(22)

ATOM 1105 CG PRO 937 ATOM 1106 C PRO 937 ATOM 1107 O PRO 937 ATOM 1108 N TYR 938 ATOM 1110 CA TYR 938 ATOM 1111 CB TYR 938 ATOM 1120 C TYR 938 ATOM 1121 O TYR 938 ATOM 1122 N LYS 939 ATOM 1124 CA LYS 939 ATOM 1125 CB LYS 939 ATOM 1126 C LYS 939 ATOM 1127 O LYS 939 ATOM 1129 CB ASP 998 ATOM 1130 C ASP 998 ATOM 1131 O ASP 998 ATOM 1134 N ASP 998 ATOM 1136 CA ASP 998 ATOM 1137 N PHE 999 ATOM 1139 CA PHE 999 ATOM 1140 CB PHE 999 ATOM 1141 CG PHE 999 ATOM 1142 CD1 PHE 999 ATOM 1143 CD2 PHE 999 ATOM 1144 CE1 PHE 999 ATOM 1145 CE2 PHE 999 ATOM 1146 CZ PHE 999 ATOM 1147 C PHE 999 ATOM 1148 O PHE 999 ATOM 1149 N LEU 1000 ATOM 1151 CA LEU 1000 ATOM 1152 CB LEU 1000 ATOM 1153 CG LEU 1000 ATOM 1154 CD1 LEU 1000 ATOM 1155 CD2 LEU 1000 ATOM 1156 C LEU 1000 ATOM 1157 O LEU 1000 ATOM 1158 N THR 1001 ATOM 1160 CA THR 1001 ATOM 1161 CB THR 1001

28.378 5.582 1.493 1.00 47.42 28.019 8.501 -0.774 1.00 53.83 28.644 9.558 -0.937 1.00 53.64 27.153 8.046 -1.660 1.00 54.91 26.918 8.803 -2.859 1.00 62.52 27.580 8.161 -4.080 1.00 67.73 25.443 8.800 -3.059 1.00 67.31 24.722 8.082 -2.361 1.00 66.13 25.027 9.601 -4.038 1.00 75.30 23.639 9.770 -4.445 1.00 81.21 23.209 11.254 -4.284 1.00 80.04 23.543 9.331 -5.921 1.00 87.24 24.582 9.384 -6.646 1.00 90.23 17.986 15.692 3.023 1.00 53.00 20.489 15.723 3.377 1.00 55.33 21.051 16.058 4.426 1.00 56.29 19.408 16.931 1.400 1.00 54.52 19.279 16.514 2.829 1.00 55.12 20.900 14.687 2.653 1.00 52.90 21.984 13.834 3.111 1.00 46.86 21.841 12.420 2.528 1.00 51.05 20.897 11.537 3.296 1.00 55.62 21.249 10.236 3.606 1.00 56.12 19.671 12.022 3.751 1.00 60.98 20.397 9.422 4.368 1.00 61.93 18.816 11.222 4.509 1.00 61.09 19.183 9.917 4.820 1.00 60.64 23.373 14.302 2.837 1.00 41.06 23.632 14.937 1.820 1.00 36.04 24.238 14.057 3.812 1.00 37.57 25.651 14.326 3.652 1.00 36.08 26.401 14.306 4.985 1.00 35.67 25.923 15.286 6.057 1.00 36.23 26.941 15.370 7.201 1.00 29.94 25.707 16.654 5.435 1.00 38.66 26.089 13.139 2.756 1.00 35.16 25.330 12.167 2.569 1.00 32.68 27.292 13.228 2.201 1.00 29.92 27.803 12.236 1.285 1.00 25.42 27.396 12.560 -0.178 1.00 30.10

FIG. 7(23)

ATOM 1162 OG1 THR 1001 ATOM 1164 CG2 THR 1001 ATOM 1165 C THR 1001 ATOM 1166 O THR 1001 ATOM 1167 N LEU 1002 ATOM 1169 CA LEU 1002 ATOM 1170 CB LEU 1002 ATOM 1171 CG LEU 1002 ATOM 1172 CD1 LEU 1002 ATOM 1173 CD2 LEU 1002 ATOM 1174 C LEU 1002 ATOM 1175 O LEU 1002 ATOM 1176 N GLU 1003 ATOM 1178 CA GLU 1003 ATOM 1179 CB GLU 1003 ATOM 1180 CG GLU 1003 ATOM 1181 CD GLU 1003 ATOM 1182 OE1 GLU 1003 ATOM 1183 OE2 GLU 1003 ATOM 1184 C GLU 1003 ATOM 1185 O GLU 1003 ATOM 1186 N HIS 1004 ATOM 1188 CA HIS 1004 ATOM 1189 CB HIS 1004 ATOM 1190 CG HIS 1004 ATOM 1191 CD2 HIS 1004 ATOM 1192 ND1 HIS 1004 ATOM 1194 CE1 HIS 1004 ATOM 1195 NE2 HIS 1004 ATOM 1197 C HIS 1004 ATOM 1198 O HIS 1004 ATOM 1199 N LEU 1005 ATOM 1201 CA LEU 1005 ATOM 1202 CB LEU 1005 ATOM 1203 CG LEU 1005 ATOM 1204 CD1 LEU 1005 ATOM 1205 CD2 LEU 1005 ATOM 1206 C LEU 1005 ATOM 1207 O LEU 1005 ATOM 1208 N ILE 1006

28.055 13.771 -0.605 1.00 33.54 25.878 12.741 -0.326 1.00 29.24 29.303 12.388 1.338 1.00 27.68 29.805 13.303 1.985 1.00 28.02 30.020 11.552 0.592 1.00 26.85 31.454 11.636 0.572 1.00 24.39 32.044 10.545 -0.298 1.00 22.71 32.269 9.304 0.573 1.00 27.80 32.727 8.142 -0.280 1.00 27.11 33.295 9.592 1.670 1.00 24.64 31.908 12.995 0.099 1.00 26.97 32.967 13.459 0.506 1.00 26.84 31.063 13.682 -0.666 1.00 27.89 31.428 15.000 -1.185 1.00 28.02 30.419 15.503 -2.208 1.00 32.50 30.988 16.624 -3.077 1.00 37.49 31.915 16.121 -4.170 1.00 38.89 33.065 15.743 -3.886 1.00 43.61 31.488 16.102 -5.331 1.00 46.97 31.591 16.044 -0.117 1.00 25.24 32.485 16.885 -0.211 1.00 26.57 30.748 15.953 0.913 1.00 23.16 30.746 16.884 2.040 1.00 19.58 29.508 16.719 2.912 1.00 19.12 28.227 17.024 2.208 1.00 23.47 27.173 17.784 2.570 1.00 23.78 27.911 16.508 0.964 1.00 27.88 26.718 16.936 0.596 1.00 20.57 26.246 17.710 1.554 1.00 23.61 31.940 16.631 2.885 1.00 21.64 32.753 17.508 3.075 1.00 25.00 32.055 15.419 3.394 1.00 23.11 33.186 15.072 4.222 1.00 23.79 33.131 13.581 4.589 1.00 24.17 32.183 13.199 5.743 1.00 27.48 31.030 14.150 5.821 1.00 25.44 31.679 11.771 5.627 1.00 22.50 34.506 15.467 3.558 1.00 20.41 35.361 16.034 4.206 1.00 21.82 34.668 15.212 2.264 1.00 19.50

FIG. 7(24)

ATOM 1210 CA ILE 1006 ATOM 1211 CB ILE 1006 ATOM 1212 CG2 ILE 1006 ATOM 1213 CG1 ILE 1006 ATOM 1214 CD1 ILE 1006 ATOM 1215 C ILE 1006 ATOM 1216 O ILE 1006 ATOM 1217 N CYS 1007 ATOM 1219 CA CYS 1007 ATOM 1220 CB CYS 1007 ATOM 1221 SG CYS 1007 ATOM 1222 C CYS 1007 ATOM 1223 O CYS 1007 ATOM 1224 N TYR 1008 ATOM 1226 CA TYR 1008 ATOM 1227 CB TYR 1008 ATOM 1228 CG TYR 1008 ATOM 1229 CD1 TYR 1008 ATOM 1230 CE1 TYR 1008 ATOM 1231 CD2 TYR 1008 ATOM 1232 CE2 TYR 1008 ATOM 1233 CZ TYR 1008 ATOM 1234 OH TYR 1008 ATOM 1236 C TYR 1008 ATOM 1237 O TYR 1008 ATOM 1238 N SER 1009 ATOM 1240 CA SER 1009 ATOM 1241 CB SER 1009 ATOM 1242 OG SER 1009 ATOM 1244 C SER 1009 ATOM 1245 O SER 1009 ATOM 1246 N PHE 1010 ATOM 1248 CA PHE 1010 ATOM 1249 CB PHE 1010 ATOM 1250 CG PHE 1010 ATOM 1251 CD1 PHE 1010 ATOM 1252 CD2 PHE 1010 ATOM 1253 CE1 PHE 1010 ATOM 1254 CE2 PHE 1010 ATOM 1255 CZ PHE 1010

35.914 15.589 1.609 1.00 18.77 36.128 14.806 0.276 1.00 16.46 37.602 14.777 -0.103 1.00 12.82 35.718 13.341 0.441 1.00 20.16 35.961 12.446 -0.834 1.00 11.88 35.998 17.136 1.377 1.00 22.88 37.113 17.730 1.431 1.00 21.25 34.854 17.788 1.108 1.00 21.47 34.860 19.240 0.909 1.00 21.66 33.522 19.825 0.431 1.00 24.87 33.760 21.544 -0.085 1.00 30.17 35.247 19.953 2.196 1.00 22.22 36.024 20.905 2.158 1.00 25.94 34.691 19.527 3.331 1.00 20.53 35.030 20.132 4.617 1.00 17.94 34.248 19.493 5.758 1.00 18.61 32.753 19.488 5.626 1.00 17.97 32.019 18.455 6.175 1.00 16.67 30.641 18.462 6.158 1.00 22.78 32.059 20.549 5.031 1.00 22.19 30.646 20.569 5.011 1.00 20.60 29.949 19.513 5.579 1.00 23.22 28.574 19.454 5.551 1.00 18.30 36.537 19.945 4.883 1.00 18.55 37.217 20.917 5.256 1.00 20.35 37.056 18.726 4.642 1.00 14.74 38.476 18.409 4.852 1.00 13.39 38.810 16.962 4.473 1.00 17.24 38.018 16.001 5.152 1.00 26.04 39.310 19.309 3.985 1.00 16.36 40.317 19.864 4.446 1.00 20.21 38.953 19.375 2.699 1.00 20.97 39.654 20.246 1.742 1.00 23.34 38.985 20.126 0.365 1.00 18.83 39.605 21.002 -0.685 1.00 17.13 38.830 21.940 -1.370 1.00 13.94 40.979 20.918 -0.968 1.00 17.85 39.410 22.804 -2.339 1.00 16.30 41.569 21.763 -1.917 1.00 17.15 40.772 22.714 -2.608 1.00 18.02

FIG. 7(25)

ATOM 1256 C PHE 1010 ATOM 1257 O PHE 1010 ATOM 1258 N GLN 1011 ATOM 1260 CA GLN 1011 ATOM 1261 CB GLN 1011 ATOM 1262 CG GLN 1011 ATOM 1263 CD GLN 1011 ATOM 1264 OE1 GLN 1011 ATOM 1265 NE2 GLN 1011 ATOM 1268 C GLN 1011 ATOM 1269 O GLN 1011 ATOM 1270 N VAL 1012 ATOM 1272 CA VAL 1012 ATOM 1273 CB VAL 1012 ATOM 1274 CG1 VAL 1012 ATOM 1275 CG2 VAL 1012 ATOM 1276 C VAL 1012 ATOM 1277 O VAL 1012 ATOM 1278 N ALA 1013 ATOM 1280 CA ALA 1013 ATOM 1281 CB ALA 1013 ATOM 1282 C ALA 1013 ATOM 1283 O ALA 1013 ATOM 1284 N LYS 1014 ATOM 1286 CA LYS 1014 ATOM 1287 CB LYS 1014 ATOM 1288 CG LYS 1014 ATOM 1289 CD LYS 1014 ATOM 1290 CE LYS 1014 ATOM 1291 NZ LYS 1014 ATOM 1295 C LYS 1014 ATOM 1296 O LYS 1014 ATOM 1297 N GLY 1015 ATOM 1299 CA GLY 1015 ATOM 1300 C GLY 1015 ATOM 1301 O GLY 1015 ATOM 1302 N MET 1016 ATOM 1304 CA MET 1016 ATOM 1305 CB MET 1016 ATOM 1306 CG MET 1016 ATOM 1307 SD MET 1016

39.688 21.746 2.242 1.00 22.02 40.749 22.390 2.298 1.00 23.00 38.535 22.271 2.643 1.00 19.25 38.418 23.640 3.159 1.00 19.07 36.980 23.945 3.480 1.00 12.84 36.117 24.005 2.270 1.00 6.53 34.713 24.371 2.659 1.00 18.81 34.490 25.382 3.347 1.00 21.22 33.760 23.525 2.302 1.00 26.88 39.262 23.894 4.394 1.00 18.28 39.840 24.982 4.543 1.00 19.80 39.270 22.934 5.319 1.00 11.82 40.110 23.063 6.500 1.00 13.54 39.825 21.936 7.528 1.00 15.67 40.686 22.107 8.795 1.00 10.56 38.370 21.948 7.901 1.00 14.92 41.618 23.068 6.068 1.00 16.72 42.448 23.782 6.665 1.00 20.48 42.001 22.291 5.051 1.00 15.90 43.401 22.352 4.602 1.00 17.77 43.732 21.206 3.638 1.00 10.59 43.685 23.755 3.963 1.00 15.74 44.764 24.302 4.139 1.00 17.49 42.718 24.342 3.244 1.00 17.18 42.866 25.706 2.665 1.00 15.11 41.557 26.152 2.020 1.00 23.73 41.146 25.474 0.748 1.00 23.57 41.963 26.033 -0.354 1.00 26.38 41.172 25.978 -1.617 1.00 38.71 42.034 26.404 -2.776 1.00 50.36 43.105 26.678 3.823 1.00 11.16 44.066 27.452 3.818 1.00 13.85 42.210 26.590 4.816 1.00 10.82 42.250 27.403 6.017 1.00 12.48 43.584 27.327 6.715 1.00 17.17 44.124 28.349 7.130 1.00 19.92 44.159 26.128 6.763 1.00 17.82 45.426 25.927 7.439 1.00 15.78 45.516 24.488 7.925 1.00 17.77 44.538 24.156 9.057 1.00 15.19 44.931 24.991 10.623 1.00 15.49

FIG. 7(26)

ATOM 1308 CE MET 1016 ATOM 1309 C MET 1016 ATOM 1310 O MET 1016 ATOM 1311 N GLU 1017 ATOM 1313 CA GLU 1017 ATOM 1314 CB GLU 1017 ATOM 1315 CG GLU 1017 ATOM 1316 CD GLU 1017 ATOM 1317 OE1 GLU 1017 ATOM 1318 OE2 GLU 1017 ATOM 1319 C GLU 1017 ATOM 1320 O GLU 1017 ATOM 1321 N PHE 1018 ATOM 1323 CA PHE 1018 ATOM 1324 CB PHE 1018 ATOM 1325 CG PHE 1018 ATOM 1326 CD1 PHE 1018 ATOM 1327 CD2 PHE 1018 ATOM 1328 CE1 PHE 1018 ATOM 1329 CE2 PHE 1018 ATOM 1330 CZ PHE 1018 ATOM 1331 C PHE 1018 ATOM 1332 O PHE 1018 ATOM 1333 N LEU 1019 ATOM 1335 CA LEU 1019 ATOM 1336 CB LEU 1019 ATOM 1337 CG LEU 1019 ATOM 1338 CD1 LEU 1019 ATOM 1339 CD2 LEU 1019 ATOM 1340 C LEU 1019 ATOM 1341 O LEU 1019 ATOM 1342 N ALA 1020 ATOM 1344 CA ALA 1020 ATOM 1345 CB ALA 1020 ATOM 1346 C ALA 1020 ATOM 1347 O ALA 1020 ATOM 1348 N SER 1021 ATOM 1350 CA SER 1021 ATOM 1351 CB SER 1021

46.642 24.894 10.658 1.00 5.63 46.625 26.321 6.618 1.00 14.62 47.680 26.667 7.163 1.00 15.76 46.487 26.208 5.305 1.00 14.65 47.552 26.608 4.384 1.00 21.43 47.177 26.195 2.947 1.00 21.43 48.162 26.622 1.878 1.00 22.82 47.634 26.421 0.436 1.00 27.12 46.457 26.769 0.141 1.00 24.95 48.418 25.927 -0.424 1.00 32.93 47.667 28.145 4.535 1.00 18.38 48.760 28.668 4.593 1.00 17.43 46.526 28.839 4.677 1.00 19.09 46.509 30.295 4.894 1.00 20.74 45.067 30.848 4.870 1.00 27.18 44.942 32.338 5.248 1.00 25.91 44.477 32.718 6.521 1.00 26.19 45.300 33.345 4.348 1.00 25.16 44.381 34.059 6.890 1.00 27.10 45.208 34.708 4.712 1.00 28.34 44.754 35.064 5.982 1.00 26.60 47.179 30.663 6.216 1.00 18.20 48.139 31.430 6.228 1.00 15.08 46.676 30.122 7.328 1.00 16.94 47.259 30.414 8.654 1.00 19.44 46.673 29.533 9.754 1.00 22.88 45.238 29.773 10.165 1.00 24.41 44.956 28.916 11.388 1.00 24.01 45.084 31.277 10.485 1.00 25.61 48.736 30.173 8.660 1.00 19.44 49.493 30.896 9.316 1.00 18.98 49.135 29.076 8.023 1.00 19.45 50.545 28.747 7.961 1.00 22.29 50.748 27.350 7.397 1.00 21.86 51.252 29.829 7.115 1.00 26.13 52.348 30.257 7.471 1.00 25.25 50.600 30.323 6.050 1.00 29.72 51.194 31.384 5.219 1.00 27.59 50.289 31.754 4.026 1.00 23.95

FIG. 7(27)

ATOM 1352 OG SER 1021 ATOM 1354 C SER 1021 ATOM 1355 O SER 1021 ATOM 1356 N ARG 1022 ATOM 1358 CA ARG 1022 ATOM 1359 CB ARG 1022 ATOM 1360 CG ARG 1022 ATOM 1361 CD ARG 1022 ATOM 1362 NE ARG 1022 ATOM 1364 CZ ARG 1022 ATOM 1365 NH1 ARG 1022 ATOM 1368 NH2 ARG 1022 ATOM 1371 C ARG 1022 ATOM 1372 O ARG 1022 ATOM 1373 N LYS 1023 ATOM 1375 CA LYS 1023 ATOM 1376 CB LYS 1023 ATOM 1377 C LYS 1023 ATOM 1378 O LYS 1023 ATOM 1379 N CYS 1024 ATOM 1381 CA CYS 1024 ATOM 1382 CB CYS 1024 ATOM 1383 SG CYS 1024 ATOM 1384 C CYS 1024 ATOM 1385 O CYS 1024 ATOM 1386 N ILE 1025 ATOM 1388 CA ILE 1025 ATOM 1389 CB ILE 1025 ATOM 1390 CG2 ILE 1025 ATOM 1391 CG1 ILE 1025 ATOM 1392 CD1 ILE 1025 ATOM 1393 C ILE 1025 ATOM 1394 O ILE 1025 ATOM 1395 N HIS 1026 ATOM 1397 CA HIS 1026 ATOM 1398 CB HIS 1026 ATOM 1399 CG HIS 1026 ATOM 1400 CD2 HIS 1026 ATOM 1401 ND1 HIS 1026

49.252 32.662 4.349 1.00 22.60 51.469 32.614 6.109 1.00 32.83 52.570 33.172 6.073 1.00 36.57 50.513 32.957 6.981 1.00 31.88 50.645 34.093 7.901 1.00 22.64 49.294 34.483 8.465 1.00 17.89 48.254 34.691 7.420 1.00 17.72 48.648 35.816 6.468 1.00 18.00 49.714 36.666 6.993 1.00 31.94 49.625 37.980 7.168 1.00 30.72 50.653 38.644 7.662 1.00 23.85 48.508 38.620 6.862 1.00 40.00 51.563 33.787 9.056 1.00 24.84 51.718 34.612 9.960 1.00 23.27 52.115 32.576 9.061 1.00 23.84 53.039 32.137 10.094 1.00 23.59 54.237 33.067 10.196 1.00 22.44 52.404 31.899 11.456 1.00 25.21 53.054 32.024 12.504 1.00 28.54 51.164 31.435 11.411 1.00 20.82 50.404 31.114 12.595 1.00 28.12 48.982 31.709 12.472 1.00 30.32 48.936 33.504 12.847 1.00 33.73 50.388 29.576 12.729 1.00 32.20 50.636 28.882 11.756 1.00 38.70 50.167 29.057 13.934 1.00 30.55 50.123 27.619 14.216 1.00 33.60 51.406 27.169 14.970 1.00 36.10 51.223 25.807 15.619 1.00 38.88 52.585 27.121 13.988 1.00 38.38 53.913 27.422 14.604 1.00 34.51 48.891 27.526 15.104 1.00 33.66 48.751 28.301 16.034 1.00 41.71 47.958 26.643 14.797 1.00 31.27 46.742 26.570 15.589 1.00 27.97 45.691 25.745 14.861 1.00 23.43 44.283 26.091 15.229 1,00 30.06 43.342 26.801 14.560 1.00 33.43 43.680 25.659 16.393 1.00 24.53

FIG. 7(28)

ATOM 1403 CE1 HIS 1026 ATOM 1404 NE2 HIS 1026 ATOM 1406 C HIS 1026 ATOM 1407 O HIS 1026 ATOM 1408 N ARG 1027 ATOM 1410 CA ARG 1027 ATOM 1411 CB ARG 1027 ATOM 1412 C ARG 1027 ATOM 1413 O ARG 1027 ATOM 1414 N ASP 1028 ATOM 1416 CA ASP 1028 ATOM 1417 CB ASP 1028 ATOM 1418 CG ASP 1028 ATOM 1419 OD1 ASP 1028 ATOM 1420 OD2 ASP 1028 ATOM 1421 C ASP 1028 ATOM 1422 O ASP 1028 ATOM 1423 N LEU 1029 ATOM 1425 CA LEU 1029 ATOM 1426 CB LEU 1029 ATOM 1427 CG LEU 1029 ATOM 1428 CD1 LEU 1029 ATOM 1429 CD2 LEU 1029 ATOM 1430 C LEU 1029 ATOM 1431 O LEU 1029 ATOM 1432 N ALA 1030 ATOM 1434 CA ALA 1030 ATOM 1435 CB ALA 1030 ATOM 1436 C ALA 1030 ATOM 1437 O ALA 1030 ATOM 1438 N ALA 1031 ATOM 1440 CA ALA 1031 ATOM 1441 CB ALA 1031 ATOM 1442 C ALA 1031 ATOM 1443 O ALA 1031 ATOM 1444 N ARG 1032 ATOM 1446 CA ARG 1032 ATOM 1447 CB ARG 1032 ATOM 1448 CG ARG 1032 ATOM 1449 CD ARG 1032

42.428 26.085 16.424 1.00 26.31 42.199 26.781 15.321 1.00 29.05 46.901 26.086 17.036 1.00 30.13 46.335 26.681 17.955 1.00 37.96 47.662 25.024 17.244 1.00 26.58 47.872 24.429 18.583 1.00 31.87 48.235 25.483 19.666 1.00 20.17 46.762 23.449 19.055 1.00 31.55 47.047 22.477 19.742 1.00 38.11 45.528 23.629 18.597 1.00 30.85 44.466 22.698 18.955 1.00 26.34 43.788 23.098 20.248 1.00 32.60 42.847 22.020 20.755 1.00 35.64 41.692 22.346 21.096 1.00 36.08 43.267 20.842 20.790 1.00 40.39 43.435 22.565 17.841 1.00 26.23 42.276 22.926 17.998 1.00 23.40 43.884 22.034 16.708 1.00 24.88 43.053 21.842 15.533 1.00 23.16 43.958 21.772 14.299 1.00 18.78 43.221 21.714 12.965 1.00 20.21 42.349 22.952 12.812 1.00 15.13 44.249 21.601 11.827 1.00 22.91 42.237 20.562 15.700 1.00 25.25 42.765 19.473 15.591 1.00 30.47 40.949 20.703 15.957 1.00 25.99 40.062 19.574 16.182 1.00 25.19 39.872 19.387 17.679 1.00 24.55 38.761 20.007 15.558 1.00 27.35 38.611 21.202 15.302 1.00 33.46 37.797 19.094 15.379 1.00 25.19 36.508 19.451 14.752 1.00 22.16 35.772 18.210 14.270 1.00 21.71 35.551 20.353 15.536 1.00 20.96 34.639 20.950 14.944 1.00 21.36 35.712 20.388 16.859 1.00 22.49 34.898 21.246 17.736 1.00 27.01 35.157 20.945 19.220 1.00 25.22 36.534 21.451 19.707 1.00 34.44 37.150 20.503 20.770 1.00 46.39

FIG. 7(29)

ATOM 1450 NE ARG 1032 ATOM 1452 CZ ARG 1032 ATOM 1453 NH1 ARG 1032 ATOM 1456 NH2 ARG 1032 ATOM 1459 C ARG 1032 ATOM 1460 O ARG 1032 ATOM 1461 N ASN 1033 ATOM 1463 CA ASN 1033 ATOM 1464 CB ASN 1033 ATOM 1465 CG ASN 1033 ATOM 1466 OD1 ASN 1033 ATOM 1467 ND2 ASN 1033 ATOM 1470 C ASN 1033 ATOM 1471 O ASN 1033 ATOM 1472 N ILE 1034 ATOM 1474 CA ILE 1034 ATOM 1475 CB ILE 1034 ATOM 1476 CG2 ILE 1034 ATOM 1477 CG1 ILE 1034 ATOM 1478 CD1 ILE 1034 ATOM 1479 C ILE 1034 ATOM 1480 O ILE 1034 ATOM 1481 N LEU 1035 ATOM 1483 CA LEU 1035 ATOM 1484 CB LEU 1035 ATOM 1485 CG LEU 1035 ATOM 1486 CD1 LEU 1035 ATOM 1487 CD2 LEU 1035 ATOM 1488 C LEU 1035 ATOM 1489 O LEU 1035 ATOM 1490 N LEU 1036 ATOM 1492 CA LEU 1036 ATOM 1493 CB LEU 1036 ATOM 1494 CG LEU 1036 ATOM 1495 CD1 LEU 1036 ATOM 1496 CD2 LEU 1036 ATOM 1497 C LEU 1036 ATOM 1498 O LEU 1036 ATOM 1499 N SER 1037 ATOM 1501 CA SER 1037

38.554 20.752 21.158 1.00 41.28 39.464 19.799 21.352 1.00 32.28 40.677 20.129 21.709 1.00 27.74 39.178 18.524 21.148 1.00 31.24 35.296 22.708 17.482 1.00 25.91 34.601 23.605 17.935 1.00 30.23 36.451 22.911 16.840 1.00 20.90 37.008 24.222 16.495 1.00 15.77 38.497 24.290 16.813 1.00 18.29 38.760 24.160 18.254 1.00 20.60 37.891 24.445 19.067 1.00 29.84 39.929 23.677 18.601 1.00 18.08 36.839 24.535 15.019 1.00 19.29 37.619 25.303 14.450 1.00 17.18 35.934 23.822 14.366 1.00 17.56 35.631 24.092 12.972 1.00 17.92 35.813 22.868 12.091 1.00 15.66 35.364 23.192 10.647 1.00 12.61 37.247 22.349 12.221 1.00 10.08 _38.312 23.384 11.994 1.00 18.10 34.147 24.381 13.075 1.00 21.87 33.410 23.592 13.669 1.00 26.72 33.711 25.524 12.575 1.00 21.91 32.311 25.883 12.670 1.00 19.45 32.190 27.310 13.181 1.00 18.73 32.102 27.454 14.691 1.00 21.53 33.019 26.518 15.456 1.00 8.66 32.391 28.881 15.016 1.00 19.34 31.700 25.764 11.316 1.00 20.15 32.377 25.977 10.310 1.00 21.51 30.429 25.390 11.275 1.00 24.13 29.745 25.237 10.006 1.00 26.96 29.027 23.882 9.909 1.00 20.57 28.149 23.631 8.681 1.00 17.23 28.877 23.617 7.360 1.00 7.53 27.566 22.306 8.900 1.00 18.85 28.827 26.432 9.755 1.00 31.45 27.953 26.794 10.557 1.00 29.93 29.094 27.061 8.628 1.00 34.52 28.410 28.248 8.215 1.00 37.11

FIG. 7(30)

ATOM 1502 CB SER 1037 ATOM 1503 OG SER 1037 ATOM 1505 C SER 1037 ATOM 1506 O SER 1037 ATOM 1507 N GLU 1038 ATOM 1509 CA GLU 1038 ATOM 1510 CB GLU 1038 ATOM 1511 CG GLU 1038 ATOM 1512 CD GLU 1038 ATOM 1513 OE1 GLU 1038 ATOM 1514 OE2 GLU 1038 ATOM 1515 C GLU 1038 ATOM 1516 O GLU 1038 ATOM 1517 N LYS 1039 ATOM 1519 CA LYS 1039 ATOM 1520 CB LYS 1039 ATOM 1521 C LYS 1039 ATOM 1522 O LYS 1039 ATOM 1523 N ASN 1040 ATOM 1525 CA ASN 1040 ATOM 1526 CB ASN 1040 ATOM 1527 CG ASN 1040 ATOM 1528 OD1 ASN 1040 ATOM 1529 ND2 ASN 1040 ATOM 1532 C ASN 1040 ATOM 1533 O ASN 1040 ATOM 1534 N VAL 1041 ATOM 1536 CA VAL 1041 ATOM 1537 CB VAL 1041 ATOM 1538 CG1 VAL 1041 ATOM 1539 CG2 VAL 1041 ATOM 1540 C VAL 1041 ATOM 1541 O VAL 1041 ATOM 1542 N VAL 1042 ATOM 1544 CA VAL 1042 ATOM 1545 CB VAL 1042 ATOM 1546 CG1 VAL 1042 ATOM 1547 CG2 VAL 1042 ATOM 1548 C VAL 1042 ATOM 1549 O VAL 1042

29.448 29.220 7.632 1.00 41.11 28.879 30.439 7.193 1.00 44.80 27.367 27.890 7.209 1.00 39.39 27.045 26.735 7.024 1.00 42.14 26.884 28.912 6.531 1.00 44.94 25.845 28.806 5.534 1.00 50.37 25.685 30.152 4.792 1.00 56.15 25.599 31.391 5.676 1.00 55.19 24.518 31.270 6.708 1.00 59.42 23.464 30.637 6.419 1.00 58.62 24.736 31.806 7.816 1.00 63.52 25.954 27.672 4.518 1.00 51.35 25.619 26.521 4.816 1.00 57.04 26.414 27.997 3.317 1.00 46.28 26.467 27.021 2.251 1.00 43.05 26.455 27.729 0.898 1.00 41.05 27.689 26.155 2.401 1.00 44.31 28.687 26.358 1.697 1.00 50.06 27.611 25.210 3.339 1.00 37.02 28.701 24.283 3.630 1.00 32.65 28.647 23.041 2.761 1.00 31.69 27.641 22.061 3.267 1.00 31.29 26.740 21.693 2.553 1.00 38.80 27.749 21.680 4.530 1.00 36.05 30.096 24.844 3.656 1.00 28.45 31.079 24.162 3.300 1.00 26.00 30.174 26.101 4.073 1.00 23.77 31.447 26.739 4.207 1.00 16.56 31.382 28.274 3.940 1.00 16.16 32.709 28.948 4.315 1.00 8.57 31.124 28.509 2.470 1.00 6.79 31.726 26.382 5.646 1.00 15.50 30.825 26.333 6.485 1.00 9.73 32.967 26.022 5.883 1.00 18.82 33.431 25.607 7.185 1.00 19.76 33.907 24.110 7.051 1.00 22.19 35.439 23.993 7.041 1.00 18.66 33.247 23.242 8.100 1.00 22.95 34.580 26.607 7.483 1.00 20.50 35.348 26.960 6.575 1.00 17.75

FIG. 7(31)

ATOM 1550 N LYS 1043 ATOM 1552 CA LYS 1043 ATOM 1553 CB LYS 1043 ATOM 1554 CG LYS 1043 ATOM 1555 CD LYS 1043 ATOM 1556 CE LYS 1043 ATOM 1557 NZ LYS 1043 ATOM 1561 C LYS 1043 ATOM 1562 O LYS 1043 ATOM 1563 N ILE 1044 ATOM 1565 CA ILE 1044 ATOM 1566 CB ILE 1044 ATOM 1567 CG2 ILE 1044 ATOM 1568 CG1 ILE 1044 ATOM 1569 CD1 ILE 1044 ATOM 1570 C ILE 1044 ATOM 1571 O ILE 1044 ATOM 1572 N CYS 1045 ATOM 1574 CA CYS 1045 ATOM 1575 CB CYS 1045 ATOM 1576 SG CYS 1045 ATOM 1577 C CYS 1045 ATOM 1578 O CYS 1045 ATOM 1579 N ASP 1046 ATOM 1581 CA ASP 1046 ATOM 1582 CB ASP 1046 ATOM 1583 CG ASP 1046 ATOM 1584 OD1 ASP 1046 ATOM 1585 OD2 ASP 1046 ATOM 1586 C ASP 1046 ATOM 1587 O ASP 1046 ATOM 1588 N PHE 1047 ATOM 1590 CA PHE 1047 ATOM 1591 CB PHE 1047 ATOM 1592 CG PHE 1047 ATOM 1593 CD1 PHE 1047 ATOM 1594 CD2 PHE 1047 ATOM 1595 CE1 PHE 1047 ATOM 1596 CE2 PHE 1047 ATOM 1597 CZ PHE 1047

34.675 27.082 8.726 1.00 18.30 35.679 28.070 9.103 1.00 17.43 34.977 29.420 9.277 1.00 17.68 34.202 29.845 8.031 1.00 19.19 33.560 31.228 8.186 1.00 26.86 33.270 31.885 6.820 1.00 18.32 34.353 32.806 6.425 1.00 22.63 36.373 27.687 10.399 1.00 18.35 35.709 27.235 11.330 1.00 17.37 37.692 27.880 10.461 1.00 17.47 38.504 27.558 11.645 1.00 21.49 40.010 27.390 11.267 1.00 20.48 40.896 27.250 12.502 1.00 15.75 40.221 26.237 10.300 1.00 14.66 41.584 26.344 9.669 1.00 12.76 38.432 28.735 12.626 1.00 30.73 38.370 29.888 12.207 1.00 31.68 38.454 28.436 13.918 1.00 38.50 38.437 29.444 14.968 1.00 48.73 37.027 29.586 15.558 1.00 50.35 36.259 28.069 16.173 1.00 59.69 39.473 29.041 16.033 1.00 54.63 39.981 27.912 15.986 1.00 54.88 39.811 29.954 16.956 1.00 64.20 40.816 29.700 18.021 1.00 69.98 40.454 28.407 18.788 1.00 72.94 41.338 28.165 20.009 1.00 75.40 40.930 28.584 21.110 1.00 77.66 42.428 27.547 19.878 1.00 75.18 42.219 29.580 17.354 1.00 74.21 43.183 29.036 17.940 1.00 74.94 42.307 30.205 16.171 1.00 75.46 43.462 30.212 15.245 1.00 71.53 42.919 30.267 13.790 1.00 72.10 41.906 31.381 13.526 1.00 71.34 42.139 32.327 12.526 1.00 74.26 40.747 31.501 14.284 1.00 69.46 41.242 33.367 12.293 1.00 70.87 39.847 32.533 14.066 1.00 67.97 40.096 33.467 13.068 1.00 71.41

FIG. 7(32)

ATOM 1598 C PHE 1047 ATOM 1599 O PHE 1047 ATOM 1601 CB ASP 1064 ATOM 1602 CG ASP 1064 ATOM 1603 OD1 ASP 1064 ATOM 1604 OD2 ASP 1064 ATOM 1605 C ASP 1064 ATOM 1606 O ASP 1064 ATOM 1609 N ASP 1064 ATOM 1611 CA ASP 1064 ATOM 1612 N ALA 1065 ATOM 1614 CA ALA 1065 ATOM 1615 CB ALA 1065 ATOM 1616 C ALA 1065 ATOM 1617 O ALA 1065 ATOM 1618 N ARG 1066 ATOM 1620 CA ARG 1066 ATOM 1621 CB ARG 1066 ATOM 1622 CG ARG 1066 ATOM 1623 CD ARG 1066 ATOM 1624 NE ARG 1066 ATOM 1626 CZ ARG 1066 ATOM 1627 NH1 ARG 1066 ATOM 1630 NH2 ARG 1066 ATOM 1633 C ARG 1066 ATOM 1634 O ARG 1066 ATOM 1635 N LEU 1067 ATOM 1637 CA LEU 1067 ATOM 1638 CB LEU 1067 ATOM 1639 CG LEU 1067 ATOM 1640 CD1 LEU 1067 ATOM 1641 CD2 LEU 1067 ATOM 1642 C LEU 1067 ATOM 1643 O LEU 1067 ATOM 1644 N PRO 1068 ATOM 1645 CD PRO 1068 ATOM 1646 CA PRO 1068 ATOM 1647 CB PRO 1068 ATOM 1648 CG PRO 1068 ATOM 1649 C PRO 1068

44.681 31.163 15.426 1.00 67.78 44.507 32.345 15.797 1.00 63.26 29.579 17.003 25.123 1.00 69.86 30.534 16.464 24.050 1.00 69.93 31.028 15.321 24.179 1.00 71.35 30.776 17.189 23.063 1.00 71.45 31.511 17.821 26.539 1.00 64.90 31.512 19.029 26.788 1.00 64.09 29.229 17.550 27.534 1.00 67.30 30.204 17.019 26.533 1.00 67.58 32.617 17.135 26.278 1.00 61.87 33.932 17.759 26.244 1.00 58.06 34.479 17.935 27.650 1.00 56.61 34.888 16.915 25.397 1.00 57.97 34.491 15.906 24.788 1.00 56.86 36.155 17.313 25.400 1.00 54.64 37.182 16.664 24.607 1.00 50.99 37.538 17.539 23.393 1.00 49.53 36.459 17.608 22.335 1.00 52.76 36.866 16.805 21.125 1.00 57.63 35.847 16.645 20.093 1.00 57.02 35.976 17.033 18.824 1.00 55.63 34.984 16.797 17.995 1.00 57.63 37.046 17.691 18.385 1.00 40.52 38.428 16.513 25.427 1.00 49.01 38.652 17.274 26.364 1.00 46.29 39.251 15.546 25.041 1.00 46.48 40.510 15.320 25.709 1.00 45.62 40.703 13.840 26.073 1.00 45.53 41.335 13.519 27.441 1.00 44.07 42.236 12.322 27.273 1.00 37.52 42.109 14.710 28.057 1.00 39.60 41.530 15.778 24.677 1.00 42.00 41.983 15.010 23.832 1.00 41.05 41.854 17.072 24.698 1.00 41.22 41.265 18.104 25.584 1.00 34.16 42.817 17.661 23.761 1.00 38.41 42.919 19.104 24.277 1.00 36.08 41.496 19.355 24.828 1.00 29.23 44.197 16.961 23.571 1.00 35.36

FIG. 7(33)

ATOM 1650 O PRO 1068 ATOM 1651 N LEU 1069 ATOM 1653 CA LEU 1069 ATOM 1654 CB LEU 1069 ATOM 1655 CG LEU 1069 ATOM 1656 CD1 LEU 1069 ATOM 1657 CD2 LEU 1069 ATOM 1658 C LEU 1069 ATOM 1659 O LEU 1069 ATOM 1660 N LYS 1070 ATOM 1662 CA LYS 1070 ATOM 1663 CB LYS 1070 ATOM 1664 CG LYS 1070 ATOM 1665 CD LYS 1070 ATOM 1666 CE LYS 1070 ATOM 1667 NZ LYS 1070 ATOM 1671 C LYS 1070 ATOM 1672 O LYS 1070 ATOM 1673 N TRP 1071 ATOM 1675 CA TRP 1071 ATOM 1676 CB TRP 1071 ATOM 1677 CG TRP 1071 ATOM 1678 CD2 TRP 1071 ATOM 1679 CE2 TRP 1071 ATOM 1680 CE3 TRP 1071 ATOM 1681 CD1 TRP 1071 ATOM 1682 NE1 TRP 1071 ATOM 1684 CZ2 TRP 1071 ATOM 1685 CZ3 TRP 1071 ATOM 1686 CH2 TRP 1071 ATOM 1687 C TRP 1071 ATOM 1688 O TRP 1071 ATOM 1689 N MET 1072 ATOM 1691 CA MET 1072 ATOM 1692 CB MET 1072 ATOM 1693 CG MET 1072 ATOM -1694 SD MET 1072 ATOM 1695 CE MET 1072 ATOM 1696 C MET 1072 ATOM 1697 O MET 1072

44.932 17.258 22.623 1.00 37.80 44.552 16.040 24.455 1.00 33.98 45.829 15.337 24.333 1.00 35.06 46.092 14.517 25.601 1.00 37.80 47.228 13.497 25.488 1.00 40.67 48.599 14.156 25.752 1.00 36.35 46.939 12.333 26.445 1.00 40.75 45.776 14.397 23.121 1.00 34.16 46.787 14.115 22.461 1.00 32.14 44.571 13.916 22.859 1.00 28.95 44.280 13.014 21.765 1.00 28.17 42.828 12.569 21.911 1.00 22.17 42.553 11.730 23.144 1.00 22.02 41.085 11.317 23.107 1.00 24.17 40.851 9.908 23.646 1.00 29.35 39.444 9.436 23.439 1.00 35.82 44.518 13.582 20.340 1.00 29.26 44.368 12.867 19.344 1.00 27.81 44.862 14.865 20.260 1.00 27.00 45.086 15.550 18.995 1.00 27.37 44.191 16.827 18.882 1.00 20.67 42.724 16.551 18.545 1.00 20.12 41.685 16.138 19.451 1.00 17.97 40.524 15.892 18.675 1.00 13.02 41.628 15.944 20.838 1.00 23.76 42.153 16.560 17.304 1.00 19.50 40.834 16.155 17.373 1.00 13.62 39.342 15.465 19.233 1.00 16.22 40.439 15.511 21.396 1.00 20.67 39.321 15.273 20.594 1.00 19.47 46.523 15.961 18.889 1.00 26.26 46.948 16.465 17.842 1.00 28.70 47.278 15.713 19.959 1.00 24.85 48.676 16.119 20.034 1.00 22.67 49.066 16.317 21.487 1.00 31.30 48.328 17.416 22.229 1.00 34.64 48.977 17.610 23.948 1.00 35.65 50.667 17.842 23.669 1.00 27.97 49.697 15.215 19.388 1.00 25.43 49.798 14.029 19.729 1.00 21.51

FIG. 7(34)

ATOM 1698 N ALA 1073 ATOM 1700 CA ALA 1073 ATOM 1701 CB ALA 1073 ATOM 1702 C ALA 1073 ATOM 1703 O ALA 1073 ATOM 1704 N PRO 1074 ATOM 1705 CD PRO 1074 ATOM 1706 CA PRO 1074 ATOM 1707 CB PRO 1074 ATOM 1708 CG PRO 1074 ATOM 1709 C PRO 1074 ATOM 1710 O PRO 1074 ATOM 1711 N GLU 1075 ATOM 1713 CA GLU 1075 ATOM 1714 CB GLU 1075 ATOM 1715 CG GLU 1075 ATOM 1716 CD GLU 1075 ATOM 1717 OE1 GLU 1075 ATOM 1718 OE2 GLU 1075 ATOM 1719 C GLU 1075 ATOM 1720 O GLU 1075 ATOM 1721 N THR 1076 ATOM 1723 CA THR 1076 ATOM 1724 CB THR 1076 ATOM 1725 OG1 THR 1076 ATOM 1727 CG2 THR 1076 ATOM 1728 C THR 1076 ATOM 1729 O THR 1076 ATOM 1730 N ILE 1077 ATOM 1732 CA ILE 1077 ATOM 1733 CB ILE 1077 ATOM 1734 CG2 ILE 1077 ATOM 1735 CG1 ILE 1077 ATOM 1736 CD1 ILE 1077 ATOM 1737 C ILE 1077 ATOM 1738 O ILE 1077 ATOM 1739 N PHE 1078 ATOM 1741-CA PHE 1078 ATOM 1742 CB PHE 1078 ATOM 1743 CG PHE 1078

50.545 15.800 18.547 1.00 25.55 51.571 15.024 17.874 1.00 29.80 52.369 15.912 16.958 1.00 22.65 52.448 14.453 18.989 1.00 34.88 52.431 14.970 20.115 1.00 39.38 53.183 13.355 18.724 1.00 36.01 53.087 12.450 17.570 1.00 31.55 54.040 12.771 19.769 1.00 36.24 54.544 11.485 19.115 1.00 34.34 53.415 11.137 18.193 1.00 31.88 55.189 13.670 20.288 1.00 37.13 55.570 13.575 21.447 1.00 34.58 55.746 14.533 19.440 1.00 37.40 56.813 15.422 19.884 1.00 40.62 57.598 15.990 18.707 1.00 33.55 56.853 16.957 17.844 1.00 39.40 55.952 16.300 16.828 1.00 43.14 55.965 15.055 16.720 1.00 49.09 55.228 17.040 16.124 1.00 44.63 56.239 16.546 20.757 1.00 42.73 56.903 17.061 21.639 1.00 44.76 54.982 16.888 20.524 1.00 46.13 54.304 17.923 21.283 1.00 46.22 52.991 18.319 20.605 1.00 43.95 53.245 18.666 19.230 1.00 46.46 52.361 19.481 21.334 1.00 43.93 53.991 17.378 22.662 1.00 47.62 54.175 18.057 23.650 1.00 52.45 53.442 16.173 22.717 1.00 47.96 53.123 15.528 23.980 1.00 46.99 52.496 14.151 23.720 1.00 46.43 52.691 13.232 24.895 1.00 46.16 51.024 14.306 23.384 1.00 44.29 50.336 13.010 23.163 1.00 46.43 54.418 15.345 24.767 1.00 51.37 54.473 15.577 25.974 1.00 52.53 55.458 14.931 24.058 1.00 53.41 56.750 14.696 24.672 1.00 58.94 57.506 13.570 23.925 1.00 60.74 56.901 12.184 24.124 1.00 57.84

FIG. 7(35)

ATOM 1744 CD1 PHE 1078 ATOM 1745 CD2 PHE 1078 ATOM 1746 CE1 PHE 1078 ATOM 1747 CE2 PHE 1078 ATOM 1748 CZ PHE 1078 ATOM 1749 C PHE 1078 ATOM 1750 O PHE 1078 ATOM 1751 N ASP 1079 ATOM 1753 CA ASP 1079 ATOM 1754 CB ASP 1079 ATOM 1755 CG ASP 1079 ATOM 1756 OD1 ASP 1079 ATOM 1757 OD2 ASP 1079 ATOM 1758 C ASP 1079 ATOM 1759 O ASP 1079 ATOM 1760 N ARG 1080 ATOM 1762 CA ARG 1080 ATOM 1763 CB ARG 1080 ATOM 1764 CG ARG 1080 ATOM 1765 CD ARG 1080 ATOM 1766 NE ARG 1080 ATOM 1768 CZ ARG 1080 ATOM 1769 NH1 ARG 1080 ATOM 1772 NH2 ARG 1080 ATOM 1775 C ARG 1080 ATOM 1776 O ARG 1080 ATOM 1777 N VAL 1081 ATOM 1779 CA VAL 1081 ATOM 1780 CB VAL 1081 ATOM 1781 CG1 VAL 1081 ATOM 1782 CG2 VAL 1081 ATOM 1783 C VAL 1081 ATOM 1784 O VAL 1081 ATOM 1785 N TYR 1082 ATOM 1787 CA TYR 1082 ATOM 1788 CB TYR 1082 ATOM -1789 CG TYR 1082-ATOM 1790 CD1 TYR 1082 ATOM 1791 CE1 TYR 1082 ATOM 1792 CD2 TYR 1082

56.068 11.612 23.169 1.00 54.09 57.127 11.483 25.298 1.00 58.64 55.478 10.380 23.381 1.00 53.82 56.539 10.254 25.514 1.00 57.20 55.711 9.703 24.555 1.00 55.07 57.574 15.981 24.767 1.00 63.98 57.433 16.738 25.736 1.00 67.06 58.356 16.274 23.724 1.00 66.97 59.215 17.472 23.678 1.00 68.09 60.225 17.402 22.501 1.00 66.89 60.174 16.082 21.714 1.00 69.02 60.254 16.156 20.474 1.00 71.23 60.089 14.980 22.308 1.00 69.71 58.434 18.806 23.599 1.00 67.74 59.011 19.848 23.266 1.00 66.85 57.137 18.747 23.926 1.00 68.20 56.173 19.858 23.898 1.00 66.60 55.997 20.496 25.279 1.00 67.64 54.529 20.758 25.638 1.00 71.26 53.823 19.481 26.096 1.00 73.66 52.364 19.610 26.226 1.00 75.75 51.642 18.981 27.157 1.00 74.86 50.321 19.134 27.211 1.00 69.96 52.247 18.212 28.060 1.00 72.78 56.305 20.920 22.801 1.00 63.93 55.861 22.069 22.955 1.00 61.93 56.863 20.510 21.667 1.00 61.30 57.034 21.413 20.545 1.00 58.53 58.202 20.951 19.584 1.00 60.54 59.304 20.266 20.370 1.00 62.35 57.701 20.043 18.455 1.00 55.04 55.713 21.481 19.771 1.00 56.90 55.052 20.452 19.560 1.00 57.43 55.287 22.699 19.435 1.00 51.51 54.078 22.909 18.641 1.00 41.08 -53.092 23.847 19.332 1.00 37.59 52.275 23.238 20.442 1.00 32.41 52.800 23.135 21.721 1.00 38.13 52.043 22.663 22.781 1.00 38.73 50.961 22.843 20.234 1.00 27.91

FIG. 7(36)

ATOM 1793 CE2 TYR 1082 ATOM 1794 CZ TYR 1082 ATOM 1795 OH TYR 1082 ATOM 1797 C TYR 1082 ATOM 1798 O TYR 1082 ATOM 1799 N THR 1083 ATOM 1801 CA THR 1083 ATOM 1802 CB THR 1083 ATOM 1803 OG1 THR 1083 ATOM 1805 CG2 THR 1083 ATOM 1806 C THR 1083 ATOM 1807 O THR 1083 ATOM 1808 N ILE 1084 ATOM 1810 CA ILE 1084 ATOM 1811 CB ILE 1084 ATOM 1812 CG2 ILE 1084 ATOM 1813 CG1 ILE 1084 ATOM 1814 CD1 ILE 1084 ATOM 1815 C ILE 1084 ATOM 1816 O ILE 1084 ATOM 1817 N GLN 1085 ATOM 1819 CA GLN 1085 ATOM 1820 CB GLN 1085 ATOM 1821 CG GLN 1085 ATOM 1822 CD GLN 1085 ATOM 1823 OE1 GLN 1085 ATOM 1824 NE2 GLN 1085 ATOM 1827 C GLN 1085 ATOM 1828 O GLN 1085 ATOM 1829 N SER 1086 ATOM 1831 CA SER 1086 ATOM 1832 CB SER 1086 ATOM 1833 OG SER 1086 ATOM 1835 C SER 1086 ATOM 1836 O SER 1086 ATOM 1837 N ASP 1087 ATOM 1839 CA ASP 1087 ATOM 1840 CB ASP 1087 ATOM 1841 CG ASP 1087 ATOM 1842 OD1 ASP 1087

50.189 22.374 21.287 1.00 33.59 50.739 22.290 22.572 1.00 36.82 50.001 21.874 23.679 1.00 39.60 54.591 23.598 17.410 1.00 34.81 55.240 24.608 17.545 1.00 33.62 54.394 22.997 16.236 1.00 34.71 54.819 23.573 14.946 1.00 30.90 56.106 22.894 14.384 1.00 29.46 55.789 21.598 13.837 1.00 30.18 57.159 22.768 15.486 1.00 21.74 53.678 23.371 13.946 1.00 27.79 52.651 22.777 14.293 1.00 28.80 53.804 23.869 12.721 1.00 24.37 52.700 23.615 11.797 1.00 27.69 52.739 24.381 10.465 1.00 28.65 51.450 25.166 10.284 1.00 29.19 53.977 25.259 10.361 1.00 37.75 55.235 24.517 9.985 1.00 46.61 52.689 22.143 11.459 1.00 26.44 51.627 21.589 11.173 1.00 24.29 53.861 21.507 11.518 1.00 25.11 53.920 20.097 11.188 1.00 24.39 55.315 19.612 10.823 1.00 27.61 55.753 20.012 9.411 1.00 33.25 54.653 19.826 8.347 1.00 34.07 53.943 20.779 8.004 1.00 41.60 54.546 18.632 7.797 1.00 28.88 53.296 19.267 12.258 1.00 23.23 52.900 18.141 11.981 1.00 25.97 53.195 19.798 13.480 1.00 20.86 52.488 19.040 14.507 1.00 18.08 53.044 19.256 15.926 1.00 20.91 52.870 20.559 16.440 1.00 21.60 50.962 19.336 14.353 1.00 20.67 50.138 18.531 14.806 1.00 13.79 50.602 20.415 13.609 1.00 18.68 49.190 20.793 13.324 1.00 11.08 49.038 22.249 12.805 1.00 21.08 48.845 23.287 13.920 1.00 23.79 49.348 24.407 13.745 1.00 31.01

FIG. 7(37)

ATOM 1843 OD2 ASP 1087 ATOM 1844 C ASP 1087 ATOM 1845 O ASP 1087 ATOM 1846 N VAL 1088 ATOM 1848 CA VAL 1088 ATOM 1849 CB VAL 1088 ATOM 1850 CG1 VAL 1088 ATOM 1851 CG2 VAL 1088 ATOM 1852 C VAL 1088 ATOM 1853 O VAL 1088 ATOM 1854 N TRP 1089 ATOM 1856 CA TRP 1089 ATOM 1857 CB TRP 1089 ATOM 1858 CG TRP 1089 ATOM 1859 CD2 TRP 1089 ATOM 1860 CE2 TRP 1089 ATOM 1861 CE3 TRP 1089 ATOM 1862 CD1 TRP 1089 ATOM 1863 NE1 TRP 1089 ATOM 1865 CZ2 TRP 1089 ATOM 1866 CZ3 TRP 1089 ATOM 1867 CH2 TRP 1089 ATOM 1868 C TRP 1089 ATOM 1869 O TRP 1089 ATOM 1870 N SER 1090 ATOM 1872 CA SER 1090 ATOM 1873 CB SER 1090 ATOM 1874 OG SER 1090 ATOM 1876 C SER 1090 ATOM 1877 O SER 1090 ATOM 1878 N PHE 1091 ATOM 1880 CA PHE 1091 ATOM 1881 CB PHE 1091 ATOM 1882 CG PHE 1091 ATOM 1883 CD1 PHE 1091 ATOM 1884 CD2 PHE 1091 ATOM 1885 CE1 PHE 1091 ATOM 1886 CE2 PHE 1091 ATOM 1887 CZ PHE 1091 ATOM 1888 C PHE 1091

48.212 23.013 14.967 1.00 28.91 48.632 19.860 12.261 1.00 11.16 47.406 19.640 12.177 1.00 12.65 49.520 19.390 11.390 1.00 9.61 49.181 18.404 10.345 1.00 13.37 50.351 18.195 9.389 1.00 15.40 50.057 17.067 8.486 1.00 14.68 50.609 19.477 8.587 1.00 10.67 48.839 17.061 11.014 1.00 13.67 47.897 16.387 10.618 1.00 15.00 49.618 16.668 12.015 1.00 12.30 49.301 15.460 12.748 1.00 12.96 50.236 15.279 13.960 1.00 16.98 49.764 14.195 14.887 1.00 18.14 50.325 12.884 15.031 1.00 18.48 49.476 12.162 15.893 1.00 20.05 51.460 12.245 14.503 1.00 22.61 48.640 14.215 15.657 1.00 18.89 48.451 12.995 16.255 1.00 19.54 49.725 10.839 16.249 1.00 20.08 51.709 10.927 14.855 1.00 17.00 50.846 10.243 15.722 1.00 23.71 47.873 15.711 13.207 1.00 14.68 46.987 14.958 12.842 1.00 20.33 47.636 16.823 13.923 1.00 18.59 46.287 17.209 14.413 1.00 15.54 46.297 18.603 15.043 1.00 12.20 47.066 18.621 16.237 1.00 18.86 45.256 17.190 13.309 1.00 16.50 44.128 16.691 13.487 1.00 18.14 45.635 17.745 12.158 1.00 23.35 44.746 17.776 10.997 1.00 20.78 45.445 18.399 9.786 1.00 17.07 44.533 18.524 8.598 1.00 21.98 43.396 19.347 8.666 1.00 17.34 -44.740 17.754 7.460 1.00 19.42 42.485 19.398 7.641 1.00 15.43 43.829 17.792 6.421 1.00 18.06 42.693 18.618 6.509 1.00 19.76 44.306 16.332 10.667 1.00 17.25

FIG. 7(38)

ATOM 1889 O PHE 1091 ATOM 1890 N GLY 1092 ATOM 1892 CA GLY 1092 ATOM 1893 C GLY 1092 ATOM 1894 O GLY 1092 ATOM 1895 N VAL 1093 ATOM 1897 CA VAL 1093 ATOM 1898 CB VAL 1093 ATOM 1899 CG1 VAL 1093 ATOM 1900 CG2 VAL 1093 ATOM 1901 C VAL 1093 ATOM 1902 O VAL 1093 ATOM 1903 N LEU 1094 ATOM 1905 CA LEU 1094 ATOM 1906 CB LEU 1094 ATOM 1907 CG LEU 1094 ATOM 1908 CD1 LEU 1094 ATOM 1909 CD2 LEU 1094 ATOM 1910 C LEU 1094 ATOM 1911 O LEU 1094 ATOM 1912 N LEU 1095 ATOM 1914 CA LEU 1095 ATOM 1915 CB LEU 1095 ATOM 1916 CG LEU 1095 ATOM 1917 CD1 LEU 1095 ATOM 1918 CD2 LEU 1095 ATOM 1919 C LEU 1095 ATOM 1920 O LEU 1095 ATOM 1921 N TRP 1096 ATOM 1923 CA TRP 1096 ATOM 1924 CB TRP 1096 ATOM 1925 CG TRP 1096 ATOM 1926 CD2 TRP 1096 ATOM 1927 CE2 TRP 1096 ATOM 1928 CE3 TRP 1096 ATOM 1929 CD1 TRP 1096 ATOM 1930 NE1 TRP 1096 ATOM 1932 CZ2.TRP 1096 ATOM 1933 CZ3 TRP 1096 ATOM 1934 CH2 TRP 1096

43.147 16.077 10.334 1.00 15.79 45.258 15.408 10.812 1.00 19.49 45.042 13.988 10.577 1.00 18.11 44.029 13.429 11.544 1.00 19.35 43.235 12.581 11.137 1.00 24.23 44.073 13.836 12.819 1.00 18.53 43.055 13.392 13.788 1.00 20.09 43.389 13.752 15.298 1.00 15.18 42.421 13.051 16.187 1.00 17.08 44.778 13.310 15.698 1.00 11.27 41.661 13.971 13.376 1.00 22.42 40.649 13.253 13.396 1.00 26.19 41.618 15.235 12.938 1.00 23.95 40.363 15.893 12.484 1.00 19.63 40.667 17.338 12.050 1.00 25.24 39.587 18.420 11.974 1.00 27.30 40.136 19.497 11.113 1.00 28.26 38.265 17.929 11.385 1.00 27.54 39.775 15.146 11.280 1.00 16.12 38.555 15.002 11.129 1.00 16.14 40.631 14.766 10.348 1.00 16.30 40.155 14.003 9.195 1.00 17.98 41.321 13.538 8.317 1.00 16.52 41.981 14.536 7.386 1.00 14.88 42.807 13.734 6.399 1.00 11.81 40.931 15.401 6.639 1.00 21.08 39.437 12.770 9.722 1.00 17.52 38.324 12.448 9.270 1.00 16.23 40.077 12.105 10.697 1.00 14.50 39.509 10.916 11.304 1.00 14.02 40.452 10.330 12.337 1.00 13.21 40.010 8.992 12.850 1.00 18.93 39.016 8.732 13.856 1.00 24.77 38.952 7.319 14.020 1.00 27.07 38.178 9.546 14.647 1.00 29.39 40.483 7.781 12.460 1.00 21.28 39.854 6.770 13.154 1.00 18.61 38.075 6.700 14.954 1.00 28.21 37.303 8.927 15.581 1.00 29.42 37.266 7.511 15.719 1.00 27.60

FIG. 7(39)

ATOM 1935 C TRP 1096 ATOM 1936 O TRP 1096 ATOM 1937 N GLU 1097 ATOM 1939 CA GLU 1097 ATOM 1940 CB GLU 1097 ATOM 1941 CG GLU 1097 ATOM 1942 CD GLU 1097 ATOM 1943 OE1 GLU 1097 ATOM 1944 OE2 GLU 1097 ATOM 1945 C GLU 1097 ATOM 1946 O GLU 1097 ATOM 1947 N ILE 1098 ATOM 1949 CA ILE 1098 ATOM 1950 CB ILE 1098 ATOM 1951 CG2 ILE 1098 ATOM 1952 CG1 ILE 1098 ATOM 1953 CD1 ILE 1098 ATOM 1954 C ILE 1098 ATOM 1955 O ILE 1098 ATOM 1956 N PHE 1099 ATOM 1958 CA PHE 1099 ATOM 1959 CB PHE 1099 ATOM 1960 CG PHE 1099 ATOM 1961 CD1 PHE 1099 ATOM 1962 CD2 PHE 1099 ATOM 1963 CE1 PHE 1099 ATOM 1964 CE2 PHE 1099 ATOM 1965 CZ PHE 1099 ATOM 1966 C PHE 1099 ATOM 1967 O PHE 1099 ATOM 1968 N SER 1100 ATOM 1970 CA SER 1100 ATOM 1971 CB SER 1100 ATOM 1972 OG SER 1100 ATOM 1974 C SER 1100 ATOM 1975 O SER 1100 ATOM 1976 N LEU 1101 ATOM 1978 CA LEU 1101 ATOM 1979 CB LEU 1101 ATOM 1980 CG LEU 1101

38.159 11.236 11.927 1.00 18.94 37.212 10.439 11.826 1.00 22.31 38.046 12.385 12.592 1.00 23.97 36.754 12.750 13.195 1.00 21.61 36.823 14.012 14.041 1.00 26.60 37.880 14.065 15.109 1.00 21.55 37.795 15.380 15.800 1.00 23.56 36.726 15.591 16.393 1.00 21.97 38.741 16.208 15.706 1.00 20.79 35.744 13.010 12.116 1.00 19.15 34.549 12.766 12.304 1.00 28.35 36.190 13.565 11.001 1.00 17.99 35.244 13.821 9.915 1.00 17.98 35.862 14.650 8.732 1.00 13.59 34.880 14.725 7.568 1.00 13.47 36.169 16.074 9.181 1.00 11.46 36.691 16.960 8.074 1.00 9.72 34.645 12.529 9.372 1.00 16.07 33.444 12.445 9.171 1.00 18.22 35.460 11.499 9.171 1.00 20.11 34.925 10.257 8.601 1.00 18.95 35.909 9.660 7.625 1.00 16.86 36.269 10.584 6.517 1.00 12.61 37.308 11.468 6.671 1.00 14.37 35.522 10.624 5.362 1.00 18.03 37.595 12.369 5.717 1.00 13.66 35.811 11.553 4.378 1.00 16.05 36.843 12.418 4.568 1.00 17.86 34.368 9.201 9.551 1.00 23.18 34.111 8.070 9.149 1.00 22.90 34.274 9.553 10.825 1.00 26.68 33.652 8.690 11.820 1.00 24.51 34.504 8.572 13.079 1.00 25.60 34.826 9.842 13.625 1.00 29.76 32.398 9.465 12.145 1.00 26.92 31.765 9.211 13.157 1.00 31.32 32.018 10.387 11.251 1.00 28.15 30.860 11.241 11.453 1.00 24.97 29.556 10.557 11.015 1.00 22.00 29.423 10.410 9.495 1.00 25.66

FIG. 7(40)

ATOM 1981 CD1 LEU 1101 ATOM 1982 CD2 LEU 1101 ATOM 1983 C LEU 1101 ATOM 1984 O LEU 1101 ATOM 1985 N GLY 1102 ATOM 1987 CA GLY 1102 ATOM 1988 C GLY 1102 ATOM 1989 O GLY 1102 ATOM 1990 N ALA 1103 ATOM 1992 CA ALA 1103 ATOM 1993 CB ALA 1103 ATOM 1994 C ALA 1103 ATOM 1995 O ALA 1103 ATOM 1996 N SER 1104 ATOM 1998 CA SER 1104 ATOM 1999 CB SER 1104 ATOM 2000 OG SER 1104 ATOM 2002 C SER 1104 ATOM 2003 O SER 1104 ATOM 2004 N PRO 1105 ATOM 2005 CD PRO 1105 ATOM 2006 CA PRO 1105 ATOM 2007 CB PRO 1105 ATOM 2008 CG PRO 1105 ATOM 2009 C PRO 1105 ATOM 2010 O PRO 1105 ATOM 2011 N TYR 1106 ATOM 2013 CA TYR 1106 ATOM 2014 CB TYR 1106 ATOM 2015 CG TYR 1106 ATOM 2016 CD1 TYR 1106 ATOM 2017 CE1 TYR 1106 ATOM 2018 CD2 TYR 1106 ATOM 2019 CE2 TYR 1106 ATOM 2020 CZ TYR 1106 ATOM 2021 OH TYR 1106 ATOM 2023 C TYR 1106 ATOM 2024 O TYR 1106 ATOM 2025 N PRO 1107 ATOM 2026 CD PRO 1107

28.060 9.866 9.127 1.00 22.23 29.632 11.768 8.829 1.00 32.30 30.771 11.779 12.888 1.00 26.64 29.793 11.552 13.580 1.00 31.34 31.828 12.446 13.336 1.00 24.93 31.836 13.057 14.650 1.00 28.61 32.129 12.293 15.917 1.00 32.38 31.647 12.693 16.950 1.00 35.69 33.004 11.291 15.876 1.00 35.95 33.354 10.500 17.060 1.00 31.27 33.515 9.041 16.672 1.00 36.15 34.625 10.972 17.747 1.00 34.29 35.382 11.788 17.190 1.00 36.92 34.886 10.417 18.934 1.00 33.11 36.087 10.744 19.715 1.00 35.13 35.906 10.422 21.207 1.00 38.40 34.719 10.964 21.765 1.00 50.36 37.216 9.852 19.249 1.00 34.54 37.039 8.640 19.167 1.00 33.44 38.395 10.434-18.963 1.00 32.93 38.678 11.877 18.972 1.00 31.54 39.571 9.693 18.513 1.00 29.88 40.633 10.781 18.465 1.00 22.24 39.883 11.965 18.079 1.00 28.04 39.919 8.659 19.582 1.00 32.54 39.480 8.795 20.731 1.00 28.79 40.700 7.648 19.196 1.00 34.52 41.148 6.564 20.085 1.00 39.62 42.374 6.994 20.896 1.00 37.66 43.496 7.566 20.059 1.00 39.50 43.690 8.957 19.976 1.00 37.50 44.655 9.518 19.143 1.00 35.61 44.315 6.739 19.293 1.00 34.54 45.305 7.290 18.446 1.00 38.80 45.466 8.686 18.373 1.00 38.23 46.412 9.240 17.520 1.00 31.37 40.022 6.128 21.016 1.00 47.24 40.100 6.296 22.247 1.00 46.94 38.947 5.570 20.431 1.00 52.30 38.880 5.234 18.996 1.00 52.76

FIG. 7(41)

ATOM 2027 CA PRO 1107 ATOM 2028 CB PRO 1107 ATOM 2029 CG PRO 1107 ATOM 2030 C PRO 1107 ATOM 2031 O PRO 1107 ATOM 2032 N GLY 1108 ATOM 2034 CA GLY 1108 ATOM 2035 C GLY 1108 ATOM 2036 O GLY 1108 ATOM 2037 N VAL 1109 ATOM 2039 CA VAL 1109 ATOM 2040 CB VAL 1109 ATOM 2041 CG1 VAL 1109 ATOM 2042 CG2 VAL 1109 ATOM 2043 C VAL 1109 ATOM 2044 O VAL 1109 ATOM 2045 N LYS 1110 ATOM 2047 CA LYS 1110 ATOM 2048 CB LYS 1110 ATOM 2049 C LYS 1110 ATOM 2050 O LYS 1110 ATOM 2051 N ILE 1111 ATOM 2053 CA ILE 1111 ATOM 2054 CB ILE 1111 ATOM 2055 CG2 ILE 1111 ATOM 2056 CG1 ILE 1111 ATOM 2057 CD1 ILE 1111 ATOM 2058 C ILE 1111 ATOM 2059 O ILE 1111 ATOM 2060 N ASP 1112 ATOM 2062 CA ASP 1112 ATOM 2063 CB ASP 1112 ATOM 2064 CG ASP 1112 ATOM 2065 OD1 ASP 1112 ATOM 2066 OD2 ASP 1112 ATOM 2067 C ASP 1112 ATOM 2068 O ASP 1112 ATOM 2069 N GLU 1113 ATOM 2071 CA GLU 1113 ATOM 2072 CB GLU 1113

37.750 5.088 21.125 1.00 55.67 37.078 4.223 20.066 1.00 55.09 37.420 4.931 18.797 1.00 52.62 38.035 4.300 22.408 1.00 60.55 38.668 3.231 22.377 1.00 60.88 37.631 4.894 23.533 1.00 62.85 37.790 4.284 24.845 1.00 63.10 39.171 3.783 25.228 1.00 61.44 39.319 3.010 26.178 1.00 63.49 40.181 4.228 24.498 1.00 58.31 41.548 3.835 24.766 1.00 55.54 42.430 4.181 23.580 1.00 54.11 43.857 3.787 23.857 1.00 51.33 41.875 3.528 22.306 1.00 54.09 42.006 4.657 25.949 1.00 57.04 41.492 5.749 26.163 1.00 57.18 42.969 4.140 26.711 1.00 59.43 43.497 4.849 27.880 1.00 60.27 43.928 3.842 28.936 1.00 63.70 44.664 5.796 27.538 1.00 60.52 45.570 5.410 26.780 1.00 61.06 44.665 7.006 28.115 1.00 58.79 45.732 7.987 27.859 1.00 60.01 45.236 9.441 27.886 1.00 63.41 44.517 9.798 26.596 1.00 58.31 44.413 9.688 29.145 1.00 69.87 44.341 11.144 29.528 1.00 75.64 46.949 7.891 28.781 1.00 58.91 47.670 8.862 28.992 1.00 59.56 47.187 6.697 29.299 1.00 60.43 48.312 6.407 30.173 1.00 56.25 48.318 4.919 30.421 1.00 59.88 48.273 4.131 29.122 1.00 67.87 47.179 3.893 28.564 1.00 71.34 49.348 3.765 28.628 1.00 72.11 49.612 6.795 29.489 1.00 54.37 49.634 7.066 28.284 1.00 50.67 50.710 6.741 30.236 1.00 55.36 52.024 7.089 29.683 1.00 55.99 53.051 7.374 30.806 1.00 58.69

FIG. 7(42)

ATOM 2073 C GLU 1113 ATOM 2074 O GLU 1113 ATOM 2075 N GLU 1114 ATOM 2077 CA GLU 1114 ATOM 2078 CB GLU 1114 ATOM 2079 CG GLU 1114 ATOM 2080 CD GLU 1114 ATOM 2081 OE1 GLU 1114 ATOM 2082 OE2 GLU 1114 ATOM 2083 C GLU 1114 ATOM 2084 O GLU 1114 ATOM 2085 N PHE 1115 ATOM 2087 CA PHE 1115 ATOM 2088 CB PHE 1115 ATOM 2089 CG PHE 1115 ATOM 2090 CD1 PHE 1115 ATOM 2091 CD2 PHE 1115 ATOM 2092 CE1 PHE 1115 ATOM 2093 CE2 PHE 1115 ATOM 2094 CZ PHE 1115 ATOM 2095 C PHE 1115 ATOM 2096 O PHE 1115 ATOM 2097 N CYS 1116 ATOM 2099 CA CYS 1116 ATOM 2100 CB CYS 1116 ATOM 2101 SG CYS 1116 ATOM 2102 C CYS 1116 ATOM 2103 O CYS 1116 ATOM 2104 N ARG 1117 ATOM 2106 CA ARG 1117 ATOM 2107 CB ARG 1117 ATOM 2108 CG ARG 1117 ATOM 2109 CD ARG 1117 ATOM 2110 NE ARG 1117 ATOM 2112 CZ ARG 1117 ATOM 2113 NH1 ARG 1117 ATOM 2116 NH2 ARG 1117 ATOM 2119 C ARG 1117 ATOM 2120 O ARG 1117 ATOM 2121 N ARG 1118

52.552 6.015 28.726 1.00 54.42 53.624 6.175 28.126 1.00 51.91 51.822 4.903 28.627 1.00 51.54 52.192 3.819 27.719 1.00 54.36 51.873 2.452 28.322 1.00 56.43 53.072 1.749 28.948 1.00 63.29 53.996 2.661 29.772 1.00 67.36 55.153 2.870 29.329 1.00 67.34 53.590 3.127 30.873 1.00 68.20 51.440 4.031 26.412 1.00 52.22 51.830 3.514 25.360 1.00 51.74 50.383 4.840 26.486 1.00 49.67 49.603 5.175 25.320 1.00 44.59 48.400 6.013 25.688 1.00 44.73 47.918 6.890 24.579 1.00 49.93 48.140 8.270 24.621 1.00 50.02 47.251 6.344 23.477 1.00 53.38 47.704 9.098 23.577 1.00 52.88 46.805 7.158 22.425 1.00 51.00 47.033 8.535 22.474 1.00 54.64 50.582 5.981 24.507 1.00 46.08 50.929 5.572 23.402 1.00 47.48 51.127 7.047 25.101 1.00 43.91 52.109 7.898 24.404 1.00 45.79 52.473 9.113 25.247 1.00 44.47 51.129 9.723 26.295 1.00 64.10 53.392 7.140 24.019 1.00 46.03 54.232 7.667 23.279 1.00 46.86 53.536 5.911 24.529 1.00 44.91 54.688 5.069 24.237 1.00 41.89 54.882 4.001 25.308 1.00 43.78 56.237 3.298 25.233 1.00 45.19 56.189 1.905 25.856 1.00 47.09 55.490 0.922 25.021 1.00 49.55 54.329 0.337 25.336 1.00 51.59 53.783 -0.547 24.506 1.00 51.49 53.695 0.649 26.461 1.00 47.17 54.370 4.389-22.927 1.00 38.98 55.156 4.455 21.996 1.00 42.49 53.206 3.751 22.860 1.00 35.52

FIG. 9(43)

ATOM 2123 CA ARG 1118 ATOM 2124 CB ARG 1118 ATOM 2125 CG ARG 1118 ATOM 2126 CD ARG 1118 ATOM 2127 NE ARG 1118 ATOM 2129 CZ ARG 1118 ATOM 2130 NH1 ARG 1118 ATOM 2133 NH2 ARG 1118 ATOM 2136 C ARG 1118 ATOM 2137 O ARG 1118 ATOM 2138 N LEU 1119 ATOM 2140 CA LEU 1119 ATOM 2141 CB LEU 1119 ATOM 2142 CG LEU 1119 ATOM 2143 CD1 LEU 1119 ATOM 2144 CD2 LEU 1119 ATOM 2145 C LEU 1119 ATOM 2146 O LEU 1119 ATOM 2147 N LYS 1120 ATOM 2149 CA LYS 1120 ATOM 2150 CB LYS 1120 ATOM 2151 CG LYS 1120 ATOM 2152 CD LYS 1120 ATOM 2153 CE LYS 1120 ATOM 2154 NZ LYS 1120 ATOM 2158 C LYS 1120 ATOM 2159 O LYS 1120 ATOM 2160 N GLU 1121 ATOM 2162 CA GLU 1121 ATOM 2163 CB GLU 1121 ATOM 2164 CG GLU 1121 ATOM 2165 CD GLU 1121 ATOM 2166 OE1 GLU 1121 ATOM 2167 OE2 GLU 1121 ATOM 2168 C GLU 1121 ATOM 2169 O GLU 1121 ATOM 2170 N GLY 1122 ATOM 2172 CA GLY 1122 ATOM 2173 C GLY 1122 ATOM 2174 O GLY 1122

52.745 3.072 21.649 1.00 36.78 51.330 2.559 21.880 1.00 31.14 51.216 1.675 23.068 1.00 34.41 49.766 1.587 23.535 1.00 45.83 48.897 0.750 22.693 1.00 53.41 47.564 0.658 22.826 1.00 55.58 46.862 -0.144 22.025 1.00 56.70 46.921 1.380 23.745 1.00 55.55 52.742 4.067 20.471 1.00 38.92 53.331 3.835 19.400 1.00 38.28 52.063 5.186 20.711 1.00 40.67 51.912 6.295 19.779 1.00 36.71 51.192 7.416 20.540 1.00 32.46 50.238 8.508 20.049 1.00 25.91 51.047 9.651 19.564 1.00 19.62 49.250 7.993 19.024 1.00 22.26 53.301 6.728 19.245 1.00 38.89 53.469 6.960 18.047 1.00 43.59 54.315 6.771 20.099 1.00 42.22 55.649 7.152 19.640 1.00 41.56 56.523 7.548 20.813 1.00 42.85 57.467 8.670 20.467 1.00 52.51 58.407 8.989 21.620 1.00 60.23 59.298 10.206 21.321 1.00 69.72 58.605 11.557 21.283 1.00 76.23 56.351 6.050 18.825 1.00 43.73 57.287 6.342 18.073 1.00 47.49 55.892 4.800 18.966 1.00 43.94 56.453 3.636 18.262 1.00 41.07 56.415 2.395 19.147 1.00 48.40 57.553 2.283 20.112 1.00 58.39 57.183 1.451 21.309 1.00 64.79 56.403 0.483 21.119 1.00 67.43 57.657 1.778 22.431 1.00 67.24 55.739 3.284 16.968 1.00 39.16 56.224 2.423 16.216 1.00 39.90 54.525 3.805 16.781 1.00 31.72 53.838 3.550 15.531 1.00.22.36 52.427 3.064 15.646 1.00 19.85 51.791 2.779 14.633 1.00 18.01

FIG. (44)

ATOM 2175 N THR 1123 ATOM 2177 CA THR 1123 ATOM 2178 CB THR 1123 ATOM 2179 OG1 THR 1123 ATOM 2181 CG2 THR 1123 ATOM 2182 C THR 1123 ATOM 2183 O THR 1123 ATOM 2184 N ARG 1124 ATOM 2186 CA ARG 1124 ATOM 2187 CB ARG 1124 ATOM 2188 CG ARG 1124 ATOM 2189 CD ARG 1124 ATOM 2190 NE ARG 1124 ATOM 2192 CZ ARG 1124 ATOM 2193 NH1 ARG 1124 ATOM 2196 NH2 ARG 1124 ATOM 2199 C ARG 1124 ATOM 2200 O ARG 1124 ATOM 2201 N MET 1125 ATOM 2203 CA MET 1125 ATOM 2204 CB MET 1125 ATOM 2205 CG MET 1125 ATOM 2206 SD MET 1125 ATOM 2207 CE MET 1125 ATOM 2208 C MET 1125 ATOM 2209 O MET 1125 ATOM 2210 N ARG 1126 ATOM 2212 CA ARG 1126 ATOM 2213 CB ARG 1126 ATOM 2214 CG ARG 1126 ATOM 2215 CD ARG 1126 ATOM 2216 NE ARG 1126 ATOM 2218 CZ ARG 1126 ATOM 2219 NH1 ARG 1126 ATOM 2222 NH2 ARG 1126 ATOM 2225 C ARG 1126 ATOM 2226 O ARG 1126 ATOM 2227 N ALA 1127 ATOM 2229 CA ALA 1127 ATOM 2230 CB ALA 1127

51.918 2.946 16.860 1.00 16.84 50.535 2.502 16.989 1.00 22.17 50.209 2.144 18.469 1.00 29.75 51.148 1.174 18.971 1.00 31.60 48.794 1.587 18.591 1.00 31.44 49.653 3.673 16.453 1.00 23.74 49.940 4.850 16.721 1.00 18.73 48.597 3.354 15.701 1.00 22.93 47.735 4.379 15.125 1.00 17.39 48.094 4.680 13.670 1.00 17.70 49.478 5.192 13.406 1.00 14.57 49.713 6.484 14.040 1.00 14.31 51.046 6.935 13.684 1.00 10.98 52.067 6.988 14.533 1.00 16.02 51.861 6.604 15.775 1.00 10.96 53.269 7.468 14.163 1.00 8.74 46.317 3.893 15.096 1.00 16.31 46.085 2.698 15.022 1.00 20.38 45.380 4.847 15.081 1.00 21.15 43.943 4.570 15.023 1.00 23.81 43.158 5.870 15.012 1.00 16.88 42.783 6.397 16.380 1.00 17.08 41.656 7.825 16.270 1.00 25.19 42.908 9.123 15.776 1.00 17.02 43.604 3.789 13.749 1.00 29.80 44.298 3.923 12.748 1.00 33.37 42.576 2.953 13.806 1.00 36.07 42.116 2.183 12.668 1.00 36.36 41.465 0.859 13.154 1.00 40.10 40.257 1.021 14.061 1.00 54.46 38.956 1.268 13.263 1.00 65.08 37.839 1.758 14.091 1.00 72.39 36.545 1.753 13.740 1.00 74.53 35.636 2.233 14.588 1.00 78.72 36.140 1.267 12.562 1.00 74.28 41.124 3.094 11.888 1.00 32.52 40.706 4.117 12.380 1.00 34.88 40.760 2.725 10.676 1.00 29.80 39.888 3.508 9.812 1.00 29.83 39.743 2.782 8.460 1.00 32.24

FIG. 7(45)

ATOM 2231 C ALA 1127 ATOM 2232 O ALA 1127 ATOM 2233 N PRO 1128 ATOM 2234 CD PRO 1128 ATOM 2235 CA PRO 1128 ATOM 2236 CB PRO 1128 ATOM 2237 CG PRO 1128 ATOM 2238 C PRO 1128 ATOM 2239 O PRO 1128 ATOM 2240 N ASP 1129 ATOM 2242 CA ASP 1129 ATOM 2243 CB ASP 1129 ATOM 2244 CG ASP 1129 ATOM 2245 OD1 ASP 1129 ATOM 2246 OD2 ASP 1129 ATOM 2247 C ASP 1129 ATOM 2248 O ASP 1129 ATOM 2249 N TYR 1130 ATOM 2251 CA TYR 1130 ATOM 2252 CB TYR 1130 ATOM 2253 CG TYR 1130 ATOM 2254 CD1 TYR 1130 ATOM 2255 CE1 TYR 1130 ATOM 2256 CD2 TYR 1130 ATOM 2257 CE2 TYR 1130 ATOM 2258 CZ TYR 1130 ATOM 2259 OH TYR 1130 ATOM 2261 C TYR 1130 ATOM 2262 O TYR 1130 ATOM 2263 N THR 1131 ATOM 2265 CA THR 1131 ATOM 2266 CB THR 1131 ATOM 2267 OG1 THR 1131 ATOM 2269 CG2 THR 1131 ATOM 2270 C THR 1131 ATOM 2271 O THR 1131 ATOM 2272 N THR 1132 ATOM 2274 CA-THR 1132 ATOM 2276 OG1 THR 1132

38.518 3.697 10.415 1.00 34.29 37.944 2.727 10.881 1.00 39.95 37.943 4.934 10.335 1.00 34.66 38.477 6.142 9.685 1.00 35.04 36.612 5.251 10.871 1.00 31.59 36.511 6.776 10.669 1.00 32.56 37.819 7.222 10.499 1.00 31.06 35.648 4.597 9.916 1.00 33.99 35.975 4.429 8.749 1.00 38.28 34.416 4.371 10.344 1.00 31.98 33.425 3.728 9.489 1.00 34.11 32.157 3.432 10.277 1.00 29.91 32.447 2.811 11.623 1.00 34.04 33.519 2.172 11.805 1.00 35.22 31.597 2.976 12.515 1.00 36.43 33.061 4.360 8.158 1.00 35.75 32.441 3.699 7.312 1.00 38.26 33.444 5.613 7.925 1.00 32.58 33.056 6.200 6.649 1.00 34.86 32.067 7.332 6.888 1.00 38.26 30.996 6.960 7.889 1.00 37.51 31.208 7.153 9.245 1.00 36.44 30.249 6.853 10.148 1.00 40.00 29.787 6.442 7.468 1.00 39.18 28.813 6.143 8.360 1.00 34.53 29.050 6.353 9.709 1.00 39.16 28.120 6.147 10.690 1.00 47.34 34.136 6.657 5.732 1.00 34.80 33.853 7.257 4.694 1.00 27.05 35.388 6.414 6.108 1.00 37.58 36.457 6.829 5.238 1.00 38.70 37.783 6.598 5.763 1.00 39.57 37.775 5.417 6.564 1.00 51.23 38.250 7.775 6.481 1.00 49.58 36.476 6.071 3.955 1.00 38.19 35.913 4.967 3.808 1.00 38.82 37.297 6.649 3.104 1.00 31.58 37.638 6.148 1.836 1.00 27.37 ATOM 2274 CA THR 1132 37.638 6.148 1.836 1.00 27.37 ATOM 2275 CB THR 1132 37.591 7.302 0.887 1.00 18.06 36.274 7.366 0.348 1.00 29.75

FIG. 9(46)

ATOM 2278 CG2 THR 1132 ATOM 2279 C THR 1132 ATOM 2280 O THR 1132 ATOM 2281 N PRO 1133 ATOM 2282 CD PRO 1133 ATOM 2283 CA PRO 1133 ATOM 2284 CB PRO 1133 ATOM 2285 CG PRO 1133 ATOM 2286 C PRO 1133 ATOM 2287 O PRO 1133 ATOM 2288 N GLU 1134 ATOM 2290 CA GLU 1134 ATOM 2291 CB GLU 1134 ATOM 2292 CG GLU 1134 ATOM 2293 CD GLU 1134 ATOM 2294 OE1 GLU 1134 ATOM 2295 OE2 GLU 1134 ATOM 2296 C GLU 1134 ATOM 2297 O GLU 1134 ATOM 2298 N MET 1135 ATOM 2300 CA MET 1135 ATOM 2301 CB MET 1135 ATOM 2302 CG MET 1135 ATOM 2303 SD MET 1135 ATOM 2304 CE MET 1135 ATOM 2305 C MET 1135 ATOM 2306 O MET 1135 ATOM 2307 N TYR 1136 ATOM 2309 CA TYR 1136 ATOM 2310 CB TYR 1136 ATOM 2311 CG TYR 1136 ATOM 2312 CD1 TYR 1136 ATOM 2313 CE1 TYR 1136 ATOM 2314 CD2 TYR 1136 ATOM 2315 CE2 TYR 1136 ATOM 2316 CZ TYR 1136 ATOM 2317 OH TYR 1136 ATOM 2319 C TYR 1136 ATOM 2320 O TYR 1136 ATOM 2321 N GLN 1137

38.528 7.126 -0.161 1.00 32.09 39.064 5.634 2.159 1.00 31.18 39.678 6.088 3.149 1.00 37.35 39.543 4.601 1.439 1.00 29.49 38.884 3.875 0.336 1.00 28.18 40.876 4.065 1.686 1.00 23.60 41.029 2.998 0.604 1.00 29.05 39.640 2.581 0.319 1.00 28.36 41.917 5.122 1.500 1.00 22.87 42.944 5.119 2.182 1.00 30.07 41.700 5.983 0.511 1.00 18.80 42.656 7.049 0.264 1.00 22.21 42.594 7.573 -1.160 1.00 26.28 41.214 7.564 -1.765 1.00 40.23 40.901 6.347 -2.617 1.00 42.05 41.727 6.004 -3.504 1.00 44.65 39.799 5.779 -2.453 1.00 44.07 42.547 8.164 1.300 1.00 21.07 43.528 8.877 1.543 1.00 20.78 41.375 8.304 1.940 1.00 20.24 41.233 9.304 2.996 1.00 16.52 39.775 9.658 3.319 1.00 17.57 39.158 10.807 2.420 1.00 15.02 40.199 12.320 2.187 1.00 20.17 40.632 12.648 3.877 1.00 13.20 41.974 8.751 4.191 1.00 20.41 42.772 9.461 4.787 1.00 25.79 41.836 7.448 4.445 1.00 20.30 42.565 6.817 5.540 1.00 17.65 42.082 5.394 5.832 1.00 21.89 42.786 4.775 7.041 1.00 26.17 42.702 5.353 8.325 1.00 20.81 43.364 4.781 9.427 1.00 17.33 43.554 3.612 6.900 1.00 26.03 44.225 3.034 7.998 1.00 12.75 44.124 3.615 9.245 1.00 16.64 44.791 2.999 10.281 1.00 17.57 44.077 6.847 5.267 1.00 14.28 44.892 7.066 6.179 1.00 19.62 44.479 6.693 4.022 1.00 12.55

FIG. 7(47)

ATOM 2323 CA GLN 1137 ATOM 2324 CB GLN 1137 ATOM 2325 CG GLN 1137 ATOM 2326 CD GLN 1137 ATOM 2327 OE1 GLN 1137 ATOM 2328 NE2 GLN 1137 ATOM 2331 C GLN 1137 ATOM 2332 O GLN 1137 ATOM 2333 N THR 1138 ATOM 2335 CA THR 1138 ATOM 2336 CB THR 1138 ATOM 2337 OG1 THR 1138 ATOM 2339 CG2 THR 1138 ATOM 2340 C THR 1138 ATOM 2341 O THR 1138 ATOM 2342 N MET 1139 ATOM 2344 CA MET 1139 ATOM 2345 CB MET 1139 ATOM 2346 CG MET 1139 ATOM 2347 SD MET 1139 ATOM 2348 CE MET 1139 ATOM 2349 C MET 1139 ATOM 2350 O MET 1139 ATOM 2351 N LEU 1140 ATOM 2353 CA LEU 1140 ATOM 2354 CB LEU 1140 ATOM 2355 CG LEU 1140 ATOM 2356 CD1 LEU 1140 ATOM 2357 CD2 LEU 1140 ATOM 2358 C LEU 1140 ATOM 2359 O LEU 1140 ATOM 2360 N ASP 1141 ATOM 2362 CA ASP 1141 ATOM 2363 CB ASP 1141 ATOM 2364 CG ASP 1141 ATOM 2365 OD1 ASP 1141 ATOM 2366 OD2 ASP 1141 ATOM 2367 C ASP 1141 ATOM 2368 O ASP 1141 ATOM 2369 N CYS 1142

45.903 6.777 3.758 1.00 16.34 46.218 6.412 2.325 1.00 18.36 47.702 6.654 1.945 1.00 21.79 48.613 5.655 2.561 1.00 14.21 48.416 4.469 2.381 1.00 22.64 49.571 6.111 3.344 1.00 18.97 46.415 8.193 4.041 1.00 20.40 47.598 8.378 4.391 1.00 25.11 45.564 9.194 3.807 1.00 18.65 45.939 10.568 4.068 1.00 15.52 44.921 11.507 3.538 1.00 19.97 44.797 11.257 2.144 1.00 18.74 45.381 12.939 3.722 1.00 21.70 46.111 10.721 5.566 1.00 12.73 47.067 11.344 6.010 1.00 18.83 45.233 10.118 6.352 1.00 9.32 45.402 10.151 7.809 1.00 12.25 44.295 9.349 8.480 1.00 13.21 42.967 10.007 8.354 1.00 5.60 41.708 8.982 9.003 1.00 17.66 40.510 9.337 7.925 1.00 2.00 46.773 9.567 8.198 1.00 15.96 47.573 10.237 8.855 1.00 17.30 47.058 8.333 7.770 1.00 15.29 48.357 7.735 8.081 1.00 14.20 48.542 6.409 7.326 1.00 6.27 47.511 5.373 7.745 1.00 15.42 47.656 4.103 6.927 1.00 8.64 47.648 5.103 9.246 1.00 14.99 49.518 8.684 7.751 1.00 17.20 50.552 8.691 8.442 1.00 18.73 49.396 9.413 6.644 1.00 20.16 50.442 10.374 6.229 1.00 19.52 50.139 10.963 4.851 1.00 20.89 50.228 9.942 3.772 1.00 25.01 50.537 8.765 4.074 1.00 30.17 49.994 10.321 2.624 1.00 26.42 50.627 11.521 7.207 1.00 15.10 51.762 11.905 7.502 1.00 8.73 49.504 12.101 7.637 1.00 10.75

FIG. 7(48)

ATOM 2371 CA CYS 1142 ATOM 2372 CB CYS 1142 ATOM 2373 SG CYS 1142 ATOM 2374 C CYS 1142 ATOM 2375 O CYS 1142 ATOM 2376 N TRP 1143 ATOM 2378 CA TRP 1143 ATOM 2379 CB TRP 1143 ATOM 2380 CG TRP 1143 ATOM 2381 CD2 TRP 1143 ATOM 2382 CE2 TRP 1143 ATOM 2383 CE3 TRP 1143 ATOM 2384 CD1 TRP 1143 ATOM 2385 NE1 TRP 1143 ATOM 2387 CZ2 TRP 1143 ATOM 2388 CZ3 TRP 1143 ATOM 2389 CH2 TRP 1143 ATOM 2390 C TRP 1143 ATOM 2391 O TRP 1143 ATOM 2392 N HIS 1144 ATOM 2394 CA HIS 1144 ATOM 2395 CB HIS 1144 ATOM 2396 CG HIS 1144 ATOM 2397 CD2 HIS 1144 ATOM 2398 ND1 HIS 1144 ATOM 2400 CE1 HIS 1144 ATOM 2401 NE2 HIS 1144 ATOM 2403 C HIS 1144 ATOM 2404 O HIS 1144 ATOM 2405 N GLY 1145 ATOM 2407 CA GLY 1145 ATOM 2408 C GLY 1145 ATOM 2409 O GLY 1145 ATOM 2410 N GLU 1146 ATOM 2412 CA GLU 1146 ATOM 2413 CB GLU 1146 ATOM 2414 CG GLU 1146 ATOM 2415 CD GLU 1146 ATOM 2416 OE1 GLU 1146 ATOM 2417 OE2 GLU 1146

49.516 13.196 8.590 1.00 13.88 48.110 13.776 8.739 1.00 17.83 47.414 14.574 7.291 1.00 17.66 50.042 12.717 9.961 1.00 15.52 50.545 13.513 10.734 1.00 16.31 49.883 11.424 10.266 1.00 20.06 50.344 10.830 11.528 1.00 17.66 49.393 9.727 11.991 1.00 15.44 48.041 10.236 12.273 1.00 14.25 46.814 9.495 12.233 1.00 18.13 45.774 10.401 12.540 1.00 12.59 46.490 8.143 11.966 1.00 16.02 47.710 11.514 12.605 1.00 7.90 46.355 11.618 12.768 1.00 13.52 44.425 10.012 12.592 1.00 8.83 45.155 7.755 12.017 1.00 11.61 44.133 8.691 12.327 1.00 16.83 51.765 10.281 11.442 1.00 23.22 52.208 9.507 12.298 1.00 27.31 52.510 10.722 10.440 1.00 24.48 53.876 10.280 10.299 1.00 26.08 54.495 10.859 9.023 1.00 19.25 55.791 10.214 8.654 1.00 18.57 56.923 10.003 9.374 1.00 14.60 56.016 9.657 7.415 1.00 19.61 57.231 9.133 7.387 1.00 19.99 57.803 9.332 8.562 1.00 15.04 54.710 10.671 11.542 1.00 32.65 54.626 11.795 12.031 1.00 31.70 55.541 9.734 12.016 1.00 37.26 56.393 9.970 13.168 1.00 31.32 57.251 11.212 13.001 1.00 35.04 57.372 11.989 13.942 1.00 38.42 57.915 11.373 11.852 1.00 34.51 58.735 12.577 11.598 1.00 37.16 59.871 12.303 10.627 1.00 37.16 61.093 11.742 11.292 1.00 50.26 61.186 10.243 11.110 1.00 54.17 61.158 9.509 12.125 1.00 55.25 61.280 9.804 9.938 1.00 59.09

FIG. 7(49)

ATOM 2418 C GLU 1146 ATOM 2419 O GLU 1146 ATOM 2420 N PRO 1147 ATOM 2421 CD PRO 1147 ATOM 2422 CA PRO 1147 ATOM 2423 CB PRO 1147 ATOM 2424 CG PRO 1147 ATOM 2425 C PRO 1147 ATOM 2426 O PRO 1147 ATOM 2427 N SER 1148 ATOM 2429 CA SER 1148 ATOM 2430 CB SER 1148 ATOM 2431 OG SER 1148 ATOM 2433 C SER 1148 ATOM 2434 O SER 1148 ATOM 2435 N GLN 1149 ATOM 2437 CA GLN 1149 ATOM 2438 CB GLN 1149 ATOM 2439 CG GLN 1149 ATOM 2440 CD GLN 1149 ATOM 2441 OE1 GLN 1149 ATOM 2442 NE2 GLN 1149 ATOM 2445 C GLN 1149 ATOM 2446 O GLN 1149 ATOM 2447 N ARG 1150 ATOM 2449 CA ARG 1150 ATOM 2450 CB ARG 1150 ATOM 2451 CG ARG 1150 ATOM 2452 CD ARG 1150 ATOM 2453 NE ARG 1150 ATOM 2455 CZ ARG 1150 ATOM 2456 NH1 ARG 1150 ATOM 2459 NH2 ARG 1150 ATOM 2462 C ARG 1150 ATOM 2463 O ARG 1150 ATOM 2464 N PRO 1151 ATOM 2465 CD PRO 1151 ATOM 2466 CA PRO 1151 ATOM 2467 CB PRO 1151 ATOM 2468 CG PRO 1151

57.910 13.742 11.052 1.00 36.46 57.378 13.665 9.934 1.00 35.72 57.861 14.868 11.791 1.00 34.09 58.490 15.147 13.099 1.00 33.72 57.082 16.020 11.336 1.00 29.77 57.446 17.106 12.351 1.00 27.86 57.668 16.334 13.619 1.00 26.72 57.436 16.417 9.922 1.00 27.04 56.559 16.784 9.158 1.00 30.21 58.698 16.255 9.551 1.00 22.56 59.177 16.616 8.210 1.00 24.23 60.707 16.724 8.203 1.00 27.40 61.314 15.477 8.545 1.00 36.19 58.743 15.674 7.101 1.00 21.41 58.890 15.964 5.913 1.00 24.41 58.272 14.508 7.485 1.00 25.45 57.831 13.547 6.497 1.00 26.28 58.224 12.142 6.946 1.00 32.79 59.705 11.907 6.958 1.00 25.96 60.279 12.196 5.622 1.00 32.77 59.765 11.744 4.591 1.00 36.63 61.312 13.007 5.604 1.00 37.86 56.327 13.670 6.278 1.00 23.40 55.783 13.145 5.306 1.00 23.12 55.662 14.339 7.215 1.00 22.72 54.226 14.581 7.132 1.00 17.86 53.721 15.243 8.392 1.00 16.38 54.161 14.532 9.598 1.00 13.96 53.285 14.903 10.728 1.00 15.08 53.632 14.090 11.879 1.00 24.55 54.066 14.564 13.040 1.00 27.63 54.192 15.871 13.230 1.00 27.18 54.423 13.717 13.991 1.00 29.34 54.025 15.559 6.008 1.00 16.82 54.913 16.382 5.715 1.00 13.09 52.873 15.464 5.320 1.00 18.01 51.793 14.453 5.320 1.00 6.32 52.726 16.442 4.240 1.00 18.95 51.489 15.948 3.492 1.00 16.01 50.726 15.092 4.520 1.00 10.59

FIG. 7(50)

ATOM 2469 C PRO 1151 ATOM 2470 O PRO 1151 ATOM 2471 N THR 1152 ATOM 2473 CA THR 1152 ATOM 2474 CB THR 1152 ATOM 2475 OG1 THR 1152 ATOM 2477 CG2 THR 1152 ATOM 2478 C THR 1152 ATOM 2479 O THR 1152 ATOM 2480 N PHE 1153 ATOM 2482 CA PHE 1153 ATOM 2483 CB PHE 1153 ATOM 2484 CG PHE 1153 ATOM 2485 CD1 PHE 1153 ATOM 2486 CD2 PHE 1153 ATOM 2487 CE1 PHE 1153 ATOM 2488 CE2 PHE 1153 ATOM 2489 CZ PHE 1153 ATOM 2490 C PHE 1153 ATOM 2491 O PHE 1153 ATOM 2492 N SER 1154 ATOM 2494 CA SER 1154 ATOM 2495 CB SER 1154 ATOM 2496 OG SER 1154 ATOM 2498 C SER 1154 ATOM 2499 O SER 1154 ATOM 2500 N GLU 1155 ATOM 2502 CA GLU 1155 ATOM 2503 CB GLU 1155 ATOM 2504 CG GLU 1155 ATOM 2505 CD GLU 1155 ATOM 2506 OE1 GLU 1155 ATOM 2507 OE2 GLU 1155 ATOM 2508 C GLU 1155 ATOM 2509 O GLU 1155 ATOM 2510 N LEU 1156 ATOM 2512 CA LEU 1156 ATOM 2513 CB LEU 1156 ATOM 2514 CG LEU 1156 ATOM 2515 CD1 LEU 1156

52.574 17.861 4.805 1.00 18.27 52.422 18.039 6.006 1.00 19.70 52.763 18.860 3.958 1.00 19.16 52.604 20.251 4.366 1.00 14.92 53.511 21.138 3.560 1.00 13.80 53.146 21.080 2.163 1.00 17.02 54.918 20.697 3.764 1.00 5.40 51.196 20.571 3.979 1.00 13.16 50.682 19.905 3.084 1.00 19.18 50.561 21.572 4.599 1.00 14.62 49.176 21.910 4.224 1.00 12.87 48.588 23.023 5.083 1.00 11.95 48.157 22.558 6.422 1.00 9.67 47.037 21.740 6.560 1.00 14.91 48.891 22.857 7.533 1.00 15.01 46.660 21.215 7.802 1.00 9.44 48.529 22.340 8.789 1.00 13.43 47.405 21.513 8.913 1.00 8.41 49.073 22.253 2.750 1.00 16.98 48.078 21.927 2.114 1.00 21.60 50.116 22.841 2.168 1.00 15.39 50.031 23.123 0.754 1.00 17.55 51.251 23.868 0.254 1.00 25.28 51.244 25.190 0.776 1.00 33.35 49.850 21.815 0.022 1.00 20.26 48.932 21.704 -0.798 1.00 23.74 50.670 20.808 0.347 1.00 19.47 50.534 19.493 -0.307 1.00 16.55 51.588 18.513 0.188 1.00 19.82 52.932 18.773 -0.486 1.00 20.20 54.128 18.210 0.249 1.00 23.11 55.226 18.377 -0.312 1.00 35.76 54.009 17.631 1.359 1.00 21.09 49.153 18.918 -0.107 1.00 16.59 48.548 18.414 -1.055 1.00.21.37 48.619 19.034 1.101 1.00 16.01 47.272 18.532 1.375 1.00 18.06 46.969 18.521 2.875 1.00 15.74 47.688 17.493 3.759 1.00 11.35 47.786 18.049 5.201 1.00 2.08

FIG. 9(51)

ATOM 2516 CD2 LEU 1156 ATOM 2517 C LEU 1156 ATOM 2518 O LEU 1156 ATOM 2519 N VAL 1157 ATOM 2521 CA VAL 1157 ATOM 2522 CB VAL 1157 ATOM 2523 CG1 VAL 1157 ATOM 2524 CG2 VAL 1157 ATOM 2525 C VAL 1157 ATOM 2526 O VAL 1157 ATOM 2527 N GLU 1158 ATOM 2529 CA GLU 1158 ATOM 2530 CB GLU 1158 ATOM 2531 CG GLU 1158 ATOM 2532 CD GLU 1158 ATOM 2533 OE1 GLU 1158 ATOM 2534 OE2 GLU 1158 ATOM 2535 C GLU 1158 ATOM 2536 O GLU 1158 ATOM 2537 N HIS 1159 ATOM 2539 CA HIS 1159 ATOM 2540 CB HIS 1159 ATOM 2541 CG HIS 1159 ATOM 2542 CD2 HIS 1159 ATOM 2543 ND1 HIS 1159 ATOM 2545 CE1 HIS 1159 ATOM 2546 NE2 HIS 1159 ATOM 2548 C HIS 1159 ATOM 2549 O HIS 1159 ATOM 2550 N LEU 1160 ATOM 2552 CA LEU 1160 ATOM 2553 CB LEU 1160 ATOM 2554 CG LEU 1160 ATOM 2555 CD1 LEU 1160 ATOM 2556 CD2 LEU 1160 ATOM 2557 C LEU 1160 ATOM 2558 O LEU 1160 ATOM 2559 N GLY 1161 ATOM 2561 CA GLY 1161 ATOM 2562 C GLY 1161

46.927 16.150 3.708 1.00 14.36 46.165 19.287 0.638 1.00 20.03 45.105 18.711 0.355 1.00 26.86 46.354 20.570 0.355 1.00 21.44 45.303 21.283 -0.362 1.00 21.15 45.513 22.801 -0.381 1.00 21.33 44.569 23.453 -1.368 1.00 15.98 45.198 23.340 0.974 1.00 13.87 45.270 20.721 -1.760 1.00 22.88 44.198 20.508 -2.333 1.00 25.54 46.445 20.400 -2.282 1.00 23.10 46.503 19.815 -3.603 1.00 27.24 47.922 19.756 -4.115 1.00 32.82 47.969 18.978 -5.404 1.00 44.73 49.187 19.268 -6.212 1.00 51.53 49.007 19.887 -7.292 1.00 54.31 50.298 18.869 -5.765 1.00 51.10 45.939 18.403 -3.643 1.00 26.42 45.167 18.051 -4.546 1.00 25.91 46.347 17.591 -2.669 1.00 26.36 45.897 16.226 -2.611 1.00 21.52 46.674 15.444 -1.576 1.00 25.28 46.322 13.991 -1.545 1.00 24.66 46.408 13.030 -2.497 1.00 24.44 45.749 13.387 -0.452 1.00 21.30 45.489 12.125 -0.731 1.00 23.16 45.879 11.884 -1.961 1.00 19.88 44.402 16.104 -2.391 1.00 21.56 43.741 15.311 -3.066 1.00 22.19 43.852 16.874 -1.456 1.00 20.25 42.408 16.832 -1.209 1.00 17.66 42.111 17.502 0.130 1.00 17.84 42.676 16.760 1.352 1.00 20.17 42.472 17.542 2.619 1.00 21.45 41.992 15.454 1.512 1.00 19.45 41.566 17.418 -2.395 1.00 17.71 40.426 17.030 -2.624 1.00 15.39 42.130 18.356 -3.153 1.00 23.52 - 41.434 18.879 -4.322 1.00 21.37 41.342 17.741 -5.346 1.00 23.91

FIG. 7(52)

ATOM 2563 O GLY 1161 ATOM 2564 N ASN 1162 ATOM 2566 CA ASN 1162 ATOM 2567 CB ASN 1162 ATOM 2568 CG ASN 1162 ATOM 2569 OD1 ASN 1162 ATOM 2570 ND2 ASN 1162 ATOM 2573 C ASN 1162 ATOM 2574 O ASN 1162 ATOM 2575 N LEU 1163 ATOM 2577 CA LEU 1163 ATOM 2578 CB LEU 1163 ATOM 2579 CG LEU 1163 ATOM 2580 CD1 LEU 1163 ATOM 2581 CD2 LEU 1163 ATOM 2582 C LEU 1163 ATOM 2583 O LEU 1163 ATOM 2584 N LEU 1164 ATOM 2586 CA LEU 1164 ATOM 2587 CB LEU 1164 ATOM 2588 CG LEU 1164 ATOM 2589 CD1 LEU 1164 ATOM 2590 CD2 LEU 1164 ATOM 2592 O LEU 1164 ATOM 2593 N GLN 1165 ATOM 2595 CA GLN 1165 ATOM 2596 CB GLN 1165 ATOM 2597 CG GLN 1165 ATOM 2598 CD GLN 1165 ATOM 2599 OE1 GLN 1165 ATOM 2600 NE2 GLN 1165 ATOM 2603 C GLN 1165 ATOM 2604 O GLN 1165 ATOM 2605 N ALA 1166 ATOM 2607 CA ALA 1166 ATOM 2608 CB ALA 1166 ATOM 2609 C ALA 1166 ATOM 2610 O ALA 1166 ATOM 2611 N ASN 1167 ATOM 2613 CA ASN 1167

40.295 17.526 -5.971 1.00 23.05 42.439 16.997 -5.520 1.00 21.49 42.428 15.854 -6.428 1.00 22.31 43.771 15.109 -6.427 1.00 22.34 44.904 15.888 -7.062 1.00 20.03 44.705 16.903 -7.701 1.00 28.17 46.117 15.401 -6.873 1.00 32.22 41.356 14.851 -5.969 1.00 23.05 40.570 14.378 -6.769 1.00 26.11 41.360 14.490 -4.688 1.00 21.05 40.405 13.523 -4.166 1.00 19.91 40.695 13.172 -2.689 1.00 19.18 41.675 12.042 -2.275 1.00 18.62 42.959 12.120 -3.020 1.00 24.35 41.983 12.043 -0.804 1.00 14.82 39.015 14.038 -4.331 1.00 19.71 38.110 13.318 -4.767 1.00 23.11 38.860 15.328 -4.121 1.00 25.91 37.533 15.941 -4.226 1.00 29.28 37.603 17.388 -3.726 1.00 31.25 36.348 18.176 -3.371 1.00 25.75 35.429 17.396 -2.435 1.00 31.52 7.018 15.866 -5.653 1.00 30.07 35.953 15.330 -5.903 1.00 32.61 37.810 16.344 -6.598 1.00 33.76 37.423 16.317 -8.003 1.00 39.95 38.451 17.048 -8.855 1.00 46.90 38.758 18.474 -8.480 1.00 49.81 39.874 19.024 -9.348 1.00 56.23 41.056 18.945 -8.997 1.00 55.97 39.508 19.536 -10.518 1.00 60.66 37.304 14.898 -8.554 1.00 39.33 36.652 14.685 -9.568 1.00 42.09 38.059 13.965 -7.988 1.00 36.82 37.994 12.586 -8.441 1.00 34.66 39.096 11.748 -7.814 1.00 32.78 36.640 12.103 -7.991 1.00 36.63 35.969 11.381 -8.713 1.00 39.47 36.226 12.532 -6.800 1.00 40.01 34.911 12.158 -6.264 1.00 42.40

FIG. 7(53)

ATOM 2614 CB ASN 1167 ATOM 2615 CG ASN 1167 ATOM 2616 OD1 ASN 1167 ATOM 2617 ND2 ASN 1167 ATOM 2620 C ASN 1167 ATOM 2621 O ASN 1167 ATOM 2622 N ALA 1168 ATOM 2624 CA ALA 1168 ATOM 2625 CB ALA 1168 ATOM 2626 C ALA 1168 ATOM 2628 O ALA 1168 ATOM 2629 O HOH ATOM 2632 O HOH ATOM 2635 O HOH ATOM 2638 O HOH ATOM 2641 O HOH 5 ATOM 2644 O HOH ATOM 2647 O HOH ATOM 2650 O HOH ATOM 2653 O HOH ATOM 2656 O HOH 10 ATOM 2659 O HOH ATOM 2662 O HOH 12 ATOM 2665 O HOH 13 ATOM 2668 O HOH ATOM 2671 O HOH 15 ATOM 2674 O HOH 16 ATOM 2677 O HOH 17 ATOM 2680 O HOH ATOM 2683 O HOH ATOM 2686 O HOH 20 ATOM 2689 O HOH 21 ATOM 2692 O. HOH 22 ATOM 2695 O HOH 23 ATOM 2698 O HOH 24 ATOM 2701 O HOH ATOM 2704 0 HOH ATOM 2707 O HOH 27 ATOM 2710 0 HOH 28 ATOM 2713 O HOH 29

34.641 12.878 -4.919 1.00 42.99 33.354 12.409 -4.242 1.00 40.80 32.306 13.046 -4.348 1.00 40.18 33.436 11.294 -3.532 1.00 36.58 33.822 12.498 -7.299 1.00 41.88 32.837 11.789 -7.391 1.00 41.83 34.057 13.558 -8.085 1.00 45.09 33.187 14.065 -9.160 1.00 46.02 32.507 12.933 -9.929 1.00 45.92 32.181 15.123 -8.728 1.00 48.61 32.627 16.233 -8.363 1.00 50.20 46.858 21.496 16.690 1.00 23.54 49.904 21.605 17.271 1.00 36.65 49.682 18.133 17.657 1.00 50.47 56.606 19.394 15.202 1.00 25.28 57.215 21.949 11.395 1.00 37.66 56.082 25.850 12.933 1.00 34.63 52.355 23.016 6.377 1.00 21.45 51.153 27.376 4.088 1.00 29.93 44.820 28.454 1.120 1.00 16.47 46.377 38.321 5.198 1.00 31.93 43.987 38.133 3.129 1.00 52.41 53.321 40.451 6.702 1.00 31.88 44.977 49.530 8.305 1.00 44.56 44.379 43.338 7.798 1.00 31.72 39.477 40.232 8.468 1.00 36.65 41.987 36.751 10.646 1.00 23.26 41.711 41.873 6.802 1.00 34.79 29.514 24.656 18.739 1.00 31.43 27.493 22.351 15.517 1.00 42.03 24.345 20.097 15.325 1.00 24.92 32.381 18.452 20.520 1.00 75.12 31.071 8.282 19.507 1.00 31.68 33.001 7.742 21.598 1.00 38.67 34.802 6.439 18.667 1.00 34.24 32.273 6.932 14.174 1.00 41.21 34.059 5.245 12.870 1.00 49.30 38.059 3.432 4.799 1.00 63.69 41.089 1.841 4.421 1.00 42.86 45.081 9.234 -0.557 1.00 39.97

FIG. 7(54)

ATOM 2716 O HOH 30	4
ATOM 2/10 0 HOLL	5
ATUM 2/19 O HOLL 32	5
ATOM 2/22 O HOLL 33	4
ATOM 2/23 0 TIOIT 34	4
ATUM 2/20 O HOW 35	
ATOM 2/31 O HOL 36	
ATOM 2/34 O HOT 37	
ATOM 2/3/ O HOZZ	
AT()M 2/40 0 11011	
ATOM 2/43 0 HOL	
ATOM 2/40 U HOLL	
ATOM 2/49 0 11011	
ATOM 2/32 0 11012	
ATOM 2/33 O HO	
ATOM 2/58 U HOLL	
ATOM 2/01 0 11011	
ATOM 2/04 O II	
ATOM 2/0/ O HOZZ	
ATOM 2//0 0 mozz	
ATOM 2//3 0 HOLL 50	
ATOM 2/10 0 HOLL	
ATOM 2/19 0 11011	
ATUM 2/02 0 110-1	
ATOM 2/03 0 11011	
ATUM 2700 O HOLL 55	
ATOM 2/91 O MOL	
A 10 M 2/34 0 11022	
AIUM ATTOM 59	
AIUM 2000 0 TOTA 50	
ATOM 2000 C TYOU 60	
AION 2000 ATOM 61	
AIUM 2007 C TROTT 62	
AIUM 2012 C TTOTT 63	
ATOM 2010 64	
AI UNI ZUIU O TYOTT 65	
ATOM 2821 O HOH 66 ATOM 2824 O HOH 66	
ATOM 2827 O HOH 67	
ATOM 2830 O HOH 68	
ATOM 2833 O HOH 69	
UT OTIT	

47.301 11.215 1.271 1.00 58.47 50.046 14.055 0.168 1.00 37.58 54.425 8.937 4.821 1.00 36.74 52.279 7.099 5.152 1.00 13.04 53.025 7.510 7.740 1.00 25.53 50.852 6.818 10.462 1.00 18.29 46.448 7.762 15.254 1.00 9.08 47.326 3.930 20.460 1.00 34.16 48.264 12.367 20.804 1.00 22.14 44.276 8.193 24.312 1.00 40.52 37.491 11.237 25.975 1.00 38.71 37.592 13.565 23.164 1.00 44.55 34.887 12.418 26.235 1.00 50.96 24.823 15.933 17.377 1.00 33.72 23.302 7.532 7.049 1.00 57.56 29.954 11.864 -3.109 1.00 38.05 42.099 3.812 18.044 1.00 40.12 38.653 0.737 18.003 1.00 37.30 34.169 14.465 16.707 1.00 20.01 37.055 32.622 16.570 1.00 31.20 29.361 31.729 15.460 1.00 21.90 25.866 31.495 10.192 1.00 24.50 23.411 32.276 10.616 1.00 68.85 22.135 37.404 8.648 1.00 40.22 28.356 36.997 10.747 1.00 22.41 29.650 33.190 8.897 1.00 31.98 34.801 35.904 3.297 1.00 59.73 24.341 20.715 4.934 1.00 28.10 37.439 20.236 25.832 1.00 33.07 32.675 51.977 19.122 1.00 33.52 32.722 54.003 14.118 1.00 25.01 29.691 54.769 22.004 1.00 27.32 21.347 47.577 14.711 1.00 27.85 25.640 44.257 7.516 1.00 24.71 24.686 40.916 3.785 1.00 55.13 33.825 48.721 10.105 1.00 39.11 39.855 54.415 18.247 1.00 50.97 36.001 50.053 7.081 1.00 68.99 37.973 50.651 5.331 1.00 32.12 40.220 53.227 6.506 1.00 15.02

FIG. 7(55)

ATOM 2836 O HOH **70** ATOM 2839 O HOH 71 ATOM 2842 O HOH 72 ATOM 2845 O HOH 73 ATOM 2848 O HOH 74 ATOM 2851 O HOH 75 ATOM 2854 O HOH 76 ATOM 2857 O HOH 77 ATOM 2860 O HOH 78 ATOM 2863 O HOH 79 ATOM 2866 O HOH 80 ATOM 2869 O HOH 81 ATOM 2872 O HOH ATOM 2875 O HOH 83 ATOM 2878 O HOH 84 85 ATOM 2881 O HOH ATOM 2884 O HOH 86 ATOM 2887 O HOH 87 ATOM 2890 O HOH 88 ATOM 2893 O HOH 89 ATOM 2896 O HOH 90 ATOM 2899 O HOH 91 ATOM 2902 O HOH 92 ATOM 2905 O HOH 93 ATOM 2908 O HOH 94 ATOM 2911 O HOH 95 ATOM 2914 O HOH 96 ATOM 2917 O HOH 97 ATOM 2920 O HOH 98 ATOM 2923 O HOH 99 ATOM 2926 O HOH 100 ATOM 2929 O HOH 101 ATOM 2932 O HOH 102 ATOM 2935 O HOH 103 ATOM 2938 O HOH 104 ATOM 2941 O HOH 105 ATOM 2944 O. HOH 106 ATOM 2947 O HOH 107 ATOM 2950 O HOH 108 ATOM 2953 O HOH 109

42.258 51.833 6.993 1.00 21.05 36.813 55.217 13.035 1.00 46.29 37.030 55.879 15.712 1.00 39.36 23.054 45.061 23.607 1.00 51.11 27.075 54.516 6.971 1.00 51.66 21.634 54.039 13.651 1.00 36.36 45.158 47.529 30.699 1.00 56.11 44.469 45.246 36.699 1.00 36.50 45.882 41.717 36.085 1.00 28.57 49.406 41.527 34.292 1.00 65.94 36.134 49.719 26.101 1.00 63.80 26.884 28.564 16.554 1.00 49.20 22.079 10.131 13.444 1.00 56.45 41.225 4.655 30.464 1.00 58.98 47.309 1.568 10.326 1.00 21.69 56.613 18.335 6.527 1.00 33.97 56.196 16.855 3.275 1.00 47.24 54.826 22.813 0.598 1.00 33.50 52.962 21.915 -2.351 1.00 66.62 47.896 24.242 -3.714 1.00 40.99 40.295 22.360 25.551 1.00 39.81 40.188 3.202 15.661 1.00 45.97 45.159 2.965 19.553 1.00 44.25 36.591 7.772 23.374 1.00 68.23 34.274 5.197 22.878 1.00 51.62 41.935 7.033 29.073 1.00 63.23 20.731 12.105 14.716 1.00 54.80 23.147 13.682 17.882 1.00 50.81 35.515 9.509 -3.558 1.00 56.70 38.933 9.503 -1.231 1.00 32.18 51.814 24.438 3.703 1.00 52.00 51.670 28.690 0.838 1.00 42.41 46.536 30.610 1.750 1.00 45.80 45.165 34.214 0.818 1.00 46.46 42.695 35.194 1.055 1.00 25.82 39.689 33.418 0.723 1.00 31.99 23.962 38.119 27.549 1.00 47.89 25.343 40.908 27.379 1.00 54.09 20.307 35.738 19.866 1.00 32.61 28.085 54.303 18.810 1.00 61.58

FIG. (56)

ATOM 2956 O HOH 110 ATOM 2959 O HOH 111 ATOM 2962 O HOH 112 ATOM 2965 O HOH 113 ATOM 2968 O HOH 114 ATOM 2971 O HOH 115 ATOM 2974 O HOH 116 ATOM 2977 O HOH 117 ATOM 2980 O HOH 118 ATOM 2983 O HOH 119 ATOM 2986 O HOH 120 ATOM 2989 O HOH 121 ATOM 2992 O HOH 122 ATOM 2995 O HOH 123 ATOM 2998 O HOH 124 ATOM 3001 O HOH 125 ATOM 3004 O HOH 126 ATOM 3007 O HOH 127 ATOM 3010 O HOH 128 ATOM 3013 O HOH 129 ATOM 3016 O HOH 130 ATOM 3019 O HOH 131 ATOM 3022 O HOH 132 ATOM 3025 O HOH 133 ATOM 3028 O HOH 134 ATOM 3031 O HOH 135 ATOM 3034 O HOH 136 ATOM 3037 O HOH 137 ATOM 3040 O HOH 138 ATOM 3043 O HOH 139 ATOM 3046 O HOH 140 ATOM 3049 O HOH 141 ATOM 3052 O HOH 142 ATOM 3055 O HOH 143 ATOM 3058 O HOH 144 ATOM 3061 O HOH 145 ATOM 3064 O HOH 146 ATOM 3067 O HOH 147 ATOM 3070 O HOH 148 ATOM 3073 O HOH 149

29.849 56.131 16.966 1.00 37.29 31.503 58.023 14.735 1.00 46.45 35.212 55.981 10.499 1.00 92.07 36.530 55.812 6.656 1.00 30.72 50.045 41.251 26.059 1.00 82.26 25.153 36.460 9.054 1.00 50.86 31.749 32.705 15.359 1.00 30.04 30.213 3.806 4.940 1.00 39.74 36.511 1.159 7.275 1.00 41.62 27.155 4.637 5.224 1.00 79.92 57.319 11.287 3.459 1.00 33.02 52.121 12.483 1.755 1.00 45.55 47.613 14.088 -5.021 1.00 41.01 57.550 26.628 16.551 1.00 30.62 32.338 10.125 23.559 1.00 35.48 31.065 5.698 3.273 1.00 42.74 32.603 4.523 1.410 1.00 33.30 34.394 2.617 4.702 1.00 42.12 37.961 10.373 -4.287 1.00 47.57 42.215 11.947 -6.970 1.00 45.13 46.307 8.952 -4.280 1.00 70.02 50.369 17.388 -3.277 1.00 42.22 47.231 21.866 22.930 1.00 50.84 45.362 17.669 27.147 1.00 48.06 27.005 23.141 18.124 1.00 49.65 45.726 12.511 -6.453 1.00 45.31 46.998 11.755 18.088 1.00 37.38 39.706 37.699 9.894 1.00 40.71 18.768 48.678 17.798 1.00 74.62 43.641 47.080 26.762 1.00 44.64 32.593 53.980 16.744 1.00 43.95 34.726 55.568 14.399 1.00 45.86 30.551 53.227 19.638 1.00 35.99 26.370 55.161 14.300 1.00 33.09 24.547 55.803 6.815 1.00 58.70 36.217 52.574 3.221 1.00 68.48 39.065 54.455 4.595 1.00 48.85 45.130 40.725 5.433 1.00 62.58 33.453 43.988 7.386 1.00 41.59 36.626 45.045 6.144 1.00 54.04

FIG. 7(57)

ATOM 3076 O HOH 150 ATOM 3079 O HOH 151 ATOM 3082 O HOH 152 ATOM 3085 O HOH 153 ATOM 3088 O HOH 154 ATOM 3091 O HOH 155 ATOM 3094 O HOH 156 ATOM 3097 O HOH 157 ATOM 3100 O HOH 158 ATOM 3103 O HOH 159 ATOM 3106 O HOH 160 ATOM 3109 O HOH 161 ATOM 3112 O HOH 162 ATOM 3115 O HOH 163 ATOM 3118 O HOH 164 ATOM 3121 O HOH 165 ATOM 3124 O HOH 166 ATOM 3127 O HOH 167 ATOM 3130 O HOH 168 ATOM 3133 O HOH 169 ATOM 3136 O HOH 170 ATOM 3139 O HOH 171 ATOM 3142 O HOH 172 ATOM 3145 O HOH 173 ATOM 3148 O HOH 174 ATOM 3151 O HOH 175 ATOM 3154 O HOH 176 ATOM 3157 O HOH 177 ATOM 3160 O HOH 178 ATOM 3163 O HOH 179 ATOM 3166 O HOH 180 ATOM 3169 O HOH 181 ATOM 3172 O HOH 182

19.458 36.977 14.386 1.00 56.50 19.502 40.993 17.850 1.00 43.35 39.793 38.257 27.760 1.00 63.31 40.730 53.944 20.682 1.00 49.91 45.371 49.402 5.710 1.00 41.53 49.114 26.038 11.482 1.00 34.43 54.085 28.403 10.828 1.00 28.60 18.729 14.990 12.752 1.00 44.66 27.500 2.046 10.138 1.00 47.88 23.505 7.763 16.082 1.00 45.49 38.101 22.326 23.406 1.00 43.42 36.788 33.961 0.261 1.00 59.95 19.380 27.777 6.595 1.00 56.29 33.583 33.343 17.339 1.00 68.25 43.221 53.467 17.853 1.00 62.89 28.154 41.110 29.042 1.00 61.19 44.877 47.914 12.583 1.00 21.27 46.589 45.908 14.329 1.00 39.48 48.235 43.490 14.297 1.00 46.88 47.834 0.528 14.762 1.00 74.55 48.711 -2.009 16.386 1.00 52.45 41.210 0.396 17.381 1.00 58.05 43.837 1.538 17.483 1.00 72.30 41.780 -2.478 14.396 1.00 47.15 31.466 11.699 21.418 1.00 45.99 35.046 14.218 20.429 1.00 39.37 22.639 26.143 4.324 1.00 36.80 26.114 24.452 6.028 1.00 31.04 28.927 30.687 4.252 1.00 41.38 23.899 6.610 18.621 1.00 56.43 53.386 11.969 4.493 1.00 39.86 30.051 43.727 0.910 1.00 47.97 31.659 49.099 8.149 1.00 52.84